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VERTICAL DISTRIBUTION OF VIBRATIONAL ENERGY OF MOLECULAR NITROGEN IN A STABLE AURORAL RED ARC AND ITS EFFECT ON IONOSPHERIC ELECTRON DENSITIES

GEORGE P. NEWTON

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GSFC — GODDARD SPACE FLIGHT CENTER —
GREENBELT, MARYLAND

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Vertical Distribution of Vibrational Energy of Molecular Nitrogen in a Stable Auroral Red Arc and its Effect on Ionospheric Electron Densities

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George P. Newton

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ABSTRACT

Previous solutions of the problem of the distribution of vibrationally excited molecular nitrogen in the thermosphere have either assumed a Boltzmann distribution and considered diffusion as one of the loss processes or solved for the energy level populations and neglected diffusion. This work combines both of the previous approaches by solving the time dependent continuity equations, including the diffusion process, for the first six energy levels of molecular nitrogen for conditions in the thermosphere corresponding to a stable auroral red arc. The primary source of molecular nitrogen excitation was subexcitation, inelastic, collisions between thermal electrons and molecular nitrogen. The reaction rates for this process were calculated from published cross section calculations. The loss processes for vibrational energy were electron and atomic oxygen quenching and vibrational energy exchange. The coupled sets of non-linear, partial differential equations were solved numerically by employing finite difference equations. The results show that molecular nitrogen in excited vibrationally to the degree that the rate constant for the rate limiting ionospheric loss process $O^+ + N_2 \rightarrow NO^+ + N$ is increased by as much as a factor of eight at F_2 region altitudes. It was found that deviations from a Boltzmann distribution caused the reaction rate constant to be as much as 1.7 times the reaction rate constant calculated for the energetically equivalent Boltzman distributed densities.

The time constant for loss of ionospheric electrons was calculated using the enhanced reaction rates. It was found that, for altitudes where the normal loss time constant is less than one day, the loss time constant was decreased in the arc by factors of 1.6 to 5 depending, on altitude. It is concluded that the observed decrease of electron density in the F_2 region in stable auroral red arcs can be explained by enhanced reaction rates for ion-atom interchange between O^+ and N_2 caused by vibrational excitation of molecular nitrogen through electronic collisions.

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CHAPTER I. INTRODUCTION

1.1 Description of Stable Auroral Red Arcs

Stable Auroral Red Arcs (SAR-Arcs) are photometrically observed enhancements of air-glow at 6300 Å and 6364 Å wavelengths occurring during geomagnetically active times. They were first observed by Barbier (1) in 1957. The emissions are from the forbidden red lines of atomic oxygen OI (^1D-^3P). Peak intensities of emissions are located at altitudes near 400 km. and vary from a few hundred rayleighs[1] to tens of kilorayleighs. The arcs generally occur near midlatitudes and are distinct in location from usual auroral phenomena. They extend over spatial dimensions of approximately 1000 km. horizontally in a meridional direction and globally in a longitudinal direction. The arcs are magnetically controlled as evidenced by their alignment in geomagnetic, rather than geographic latitude, and by their simultaneous occurrence at magnetically conjugate points. Once the SAR-arc is formed it generally persists for ten hours or longer. The frequency of observation appears to follow the solar cycle. Reviews of the general properties of SAR-arcs and citations to the literature are contained in Reference (2) and more recently Reference (3).

1.2 Cause of SAR-Arcs

The absence of the atomic oxygen green line OI (^1S-^1D) in the air glow enhancements during SAR-arcs, implies that a low energy source must exist for the excitation of the OI(^1D) state. Several mechanisms have been proposed for selectively exciting ^1D level and their implications studied (see (3) for summary)

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[1] a rayleigh is 10^6 photons cm^{-2} sec^{-1}

but one proposal has recently gained prominence. In this proposal (4) energy originating in the solar wind is transferred through the ring current in the magnetosphere to the ambient plasma, from which it is conducted down magnetic field lines into the ionosphere where it heats ambient electrons. These heated electrons collisionally excite the atomic oxygen ^1D level, but lack sufficient energy to excite the ^1S level. This proposal was utilized together with in-situ measurements of electron temperatures and densities by Roble et al. (5), (6) who found it to be consistent with all observations. Other proposals have been excluded by in-situ measurements (see (3) for discussion of the proposals and (7), (8) for observations).

1.3 Ionospheric Behavior in a SAR-ARC

From ground based (see (3) for review) and more importantly from satellite obtained data (9), (6), (7), (8), the following behavior of the ionosphere in the vicinity of SAR-arc has been determined.

At the satellites where the electron temperatures, and in some instances the ion temperatures, were measured a general enhancement of the charged particle temperatures was observed on the geomagnetic field lines intersecting the SAR-arcs. The electron densities at these satellite attitudes (usually greater than 1000 km.) showed for different SAR-arc occurrences both increases, decreases and no change in the electron densities, apparently depending on the altitude of measurement. However, corresponding topside sounder data always showed electron density depressions in the lower F_2 regions (near 300-800 km altitude) in the corresponding region of enhanced electron temperature. The electron density scale heights often are less in the red arc region, reflecting changes in the ion composition (7), (6). The more complex electron density behavior at the

higher altitudes (1000 km and greater) may in part be explained by a combination of the ion composition changes and the increased plasma temperature. A typical observation of the electron density and temperature in the vicinity of a SAR-arc is shown in Figure 1-1.

1.4 Objective of this work

One of the primary loss processes for ionization in the F_2 region, where atomic oxygen ions are the dominate ion species, is

$$O^+ + N_2 \xrightarrow{k} NO^+ + N \qquad (1\text{-}1)$$

followed by

$$NO^+ + e \xrightarrow{\alpha} N + O \qquad (1\text{-}2)$$

where k and α are the ion-atom interchange and dissociative recombination reaction rates, respectively. Typically α is about four orders of magnitude greater than k, (11), so that the rate determining process for ionization loss is reaction (1-1). However, k in reaction (1-1) is known to be a strong function of the vibrational temperature of molecular nitrogen (12), (13). This is why knowledge of the energy distribution of the excited levels plays a crucial role in the understanding of the electron loss rates in the SAR-arc. Thus, as suggested earlier, (12), the loss of ionospheric ionization may be considerably enhanced by the presence of vibrationally excited nitrogen. The source of the vibrationally excited nitrogen molecules is sub-excitation,[2] inelastic, collisions between the

[2] Subexcitation means that the final state of the N_2 is neither electronically excited nor ionized.

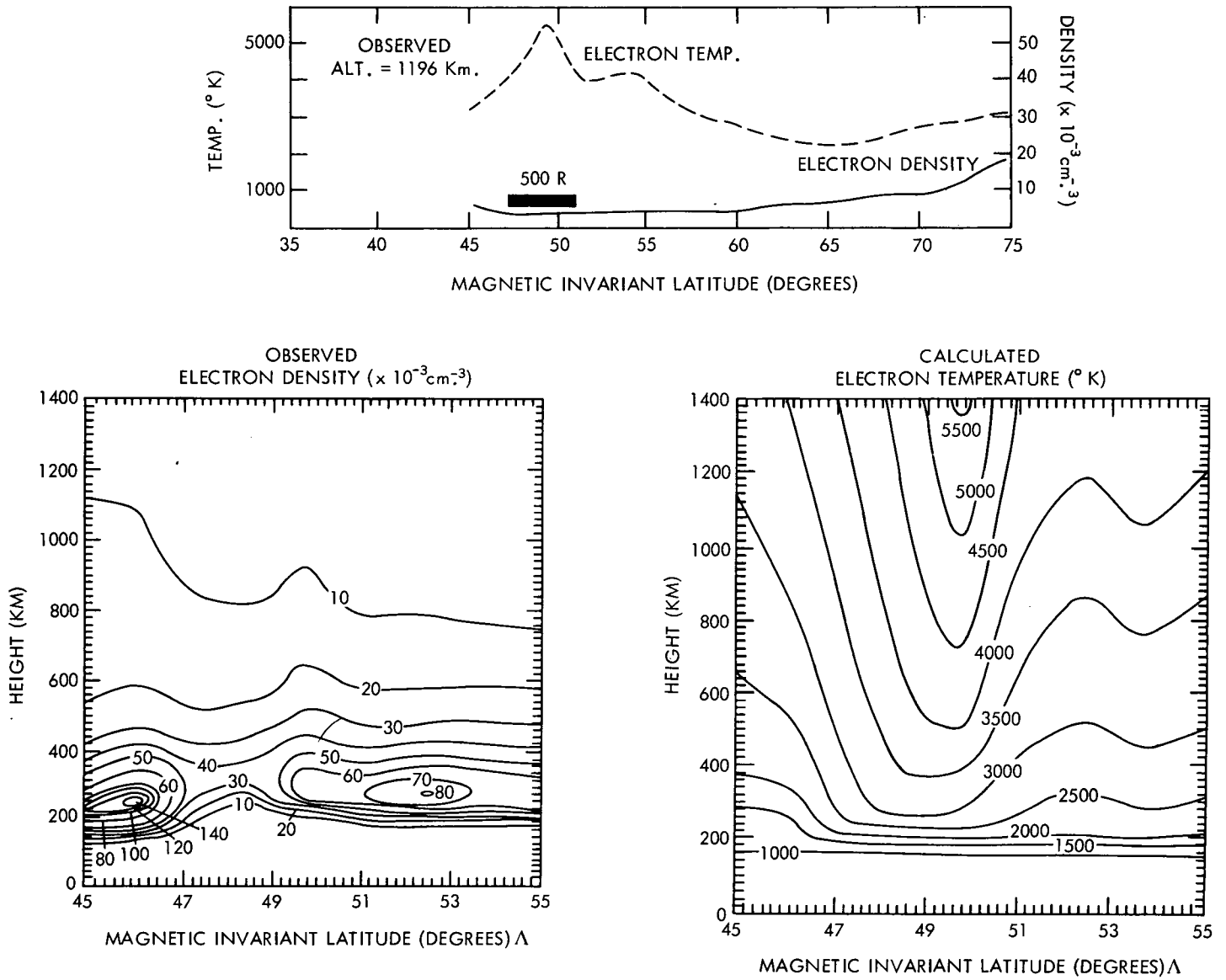

Figure 1-1. Observed ionospheric electron densities and observed and calculated electron temperatures for a 500 R SAR-arc

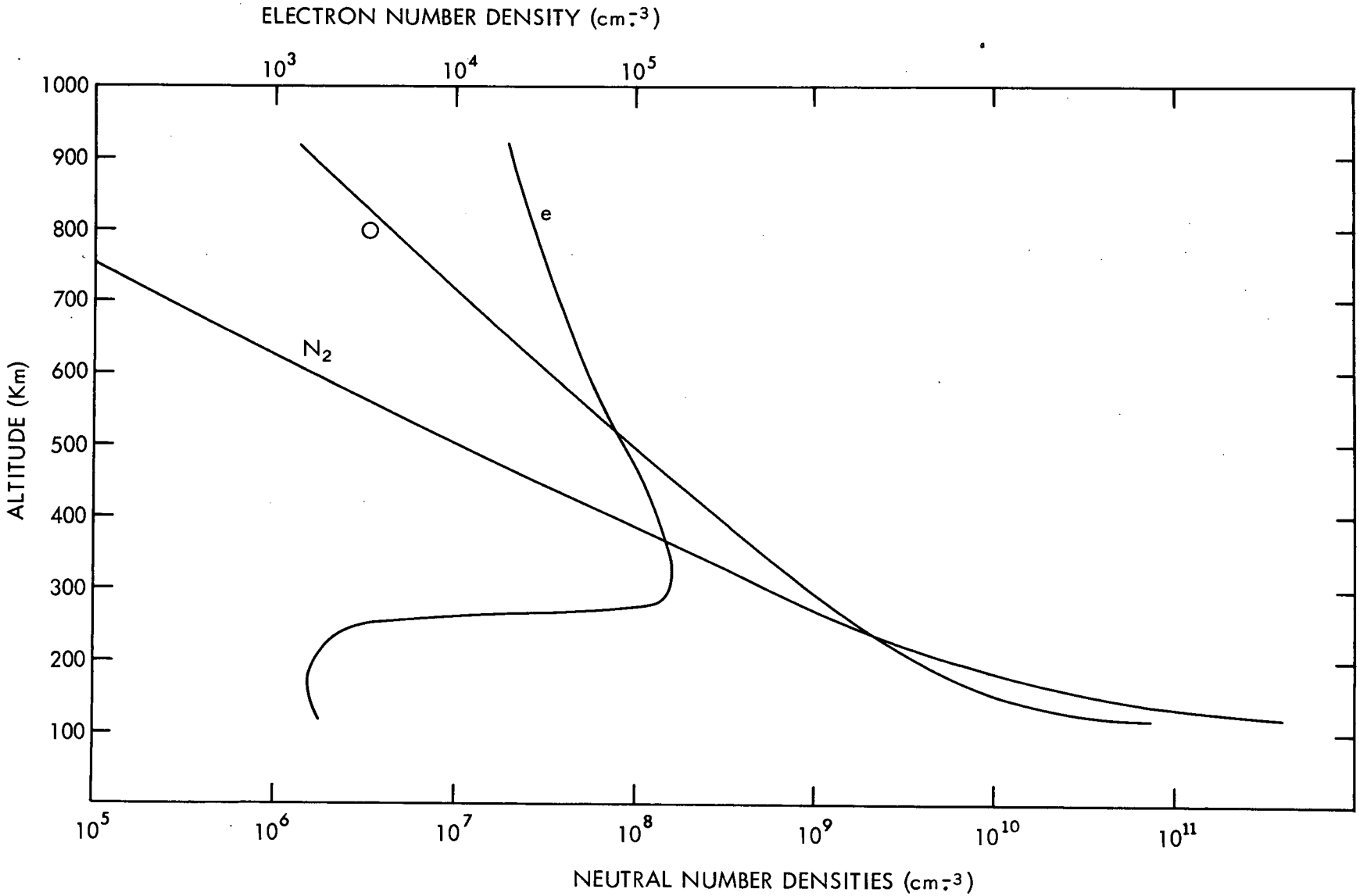

Figure 1-2. Model neutral atmosphere and ionospheric electron densities

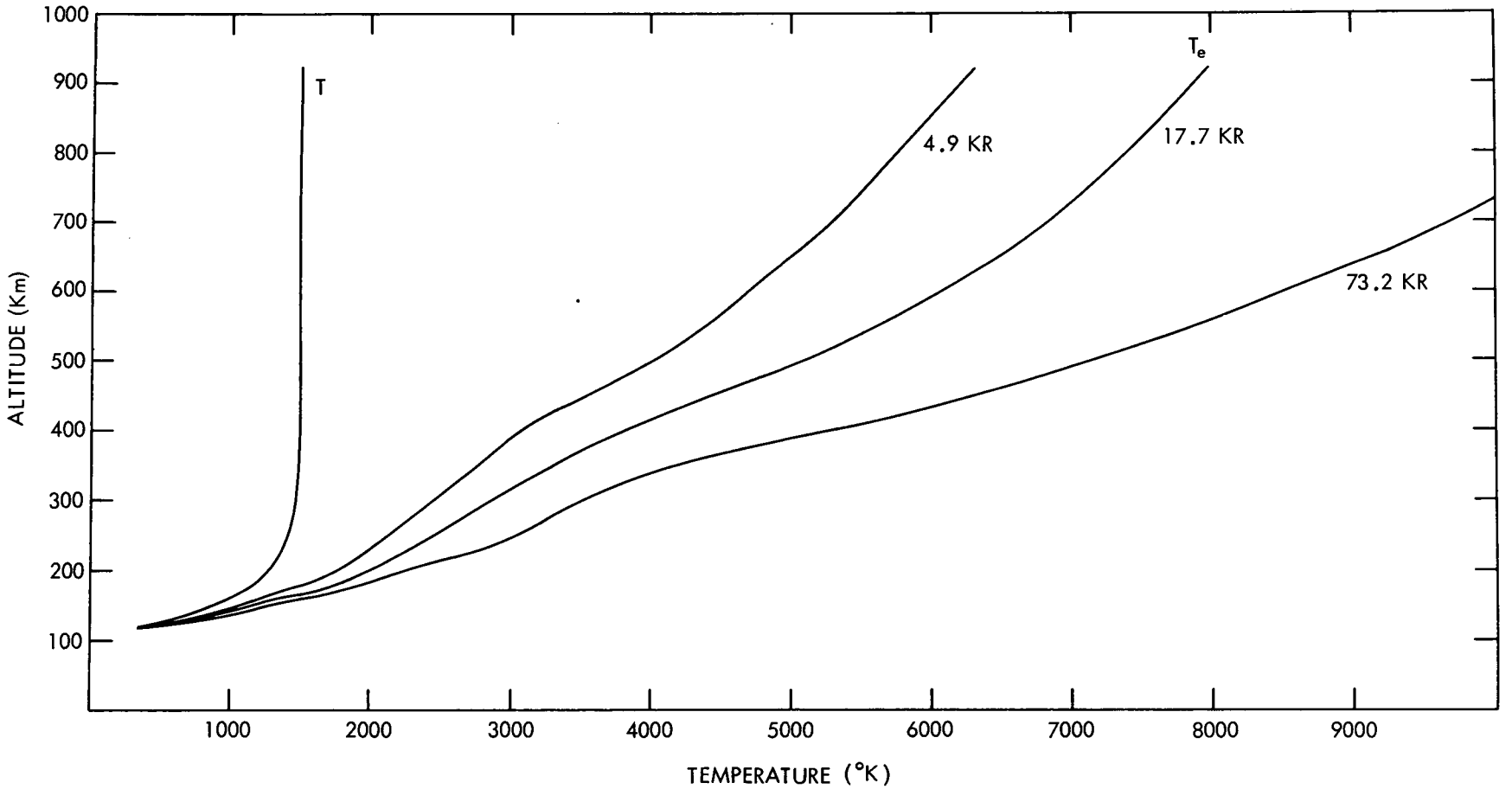

Figure 1-3. Neutral atmosphere kinetic and electron temperature models

ambient molecular nitrogen and the thermal ionospheric electrons, the same mechanism that excites the OI(^{1}D). The cross section for this type of process is important to this study (Appendix I).

The objective of this work is to investigate the distribution of vibrationally excited molecular nitrogen under conditions corresponding to a SAR-ARC to determine if the presence of vibrationally excited nitrogen can account for the observed decrease in the electron density in the F_2 region. For this study we used the same electron density profiles that Roble (10) used to calculate the temperature profiles for SAR-arcs, and we used his calculated electron temperatures. The electron density profile and model atmosphere used for this work are shown in Figure 1-2. The neutral atmospheric model used for this work is the 1965 Jacchia model (14) with an exospheric temperature of 1500°K. We did not include minor constituents. The neutral atmosphere temperature profile is shown in Figure 1-3, together with several of Robel's, (10), electron temperature profiles corresponding to different SAR-ARC intensities.

CHAPTER II. FORMULATION OF THE PROBLEM

2.1 Previous Calculations of the Distribution of Vibrationally Excited Nitrogen

Several authors have suggested that vibrationally excited nitrogen may influence the excitation of atmospheric radiations, chemical reactions, and the ionospheric temperature (15), (16), (17), (18), (12), (19). Walker et. al. (20) were the first to calculate the altitudinal distribution and diurnal variation of the vibrating molecules assuming a Boltzmann distribution. The diurnal calculations assumed an unperturbed atmosphere and ionosphere. They considered diffusion of the vibrationally excited nitrogen vertically and limited their calculation to altitudes between 100 km and 300 km altitude. They found that vibrational energy exchange with CO_2 was the dominant loss process for vibrational quanta below 125 km altitude. The principal sources of vibrational quanta in the lower thermosphere (100 km and 600 km) were found to be: (1) the reaction between atomic nitrogen and nitric oxide; (2) the collisions of photoelectrons and nitrogen molecules; and (3) possibly the quenching of metastable oxygen atoms, OI (^{1}D), by nitrogen, although the vibrational yield of the last process is unknown.

Recently, McNeal, et. al. (21) measured the reaction rate for vibrational-translation energy exchange between atomic oxygen and vibrationally excited molecular nitrogen at 300°K and found the rate to be considerably larger than extrapolated values (which were used by Walker et. al. (20).) obtained from experiments at higher temperatures. The quenching of vibrationally excited molecular nitrogen by atomic oxygen, which was ignored in the calculations of Walker et. al. (20), has been included in the calculations of Breig, et. al (22) who used the recently determined reaction rate. They essentially repeated the calculations

of Walker, et. al. (19) and found that inclusion of the loss of vibrational excitation by nitrogen molecules to atomic oxygen significantly decreased (by factors of 2 to 4) the vibrational temperatures in the lower thermosphere.

Schunk and Hays (23) solved the continuity equations for the first eleven energy levels of molecular nitrogen for altitudes above 150 km. under conditions corresponding to an aurora. Diffusion processes were not included in their calculations. The source of vibrational excitation was non-thermal electrons and the only loss process included for each level was vibrational energy exchange between nitrogen molecules. They found that when the non-thermal electron source was acting, the N_2 vibrational distribution was non-Boltzmann and that the deviation from the Boltzmann distribution increased with increasing altitude. They found that the loss rate for O^+ due to reaction (1-1) was increased by a factor of 1.5 when allowance was made for the non-Boltzmann distribution. The non-thermal electron source was allowed to operate for 15 min. and they found that the enhanced loss rate persisted for 1000-2000 sec. after the auroral bombardment commenced.

Walker (24) discussed the result of Schunk and Hays (23) and included in his discussion the effects of diffusion. He starts with the steady state continuity equation for each level and ignores quenching processes for the vibrationally excited nitrogen molecules. Under these conditions, the source of vibrational excitation and diffusion are the only terms which can cause departures from a Boltzmann distribution. By comparing the production term for a given vibrational level with the production at that level due to vibrational exchange, he concluded that departures for vibrational levels containing a significant fraction of the nitrogen molecules will not exist at altitudes below 300 km. By comparing the diffusive

flux term with the loss due to vibrational energy exchange he concludes that diffusion is less important than vibrational energy exchange at altitudes below 370 km. These conclusions were based on conditions of an undisturbed atmosphere and source terms similar to those used by Walker, et al. (20).

2.2 Differences between this and previous works.

The source of vibrational excitation for this work is the thermal electrons in SAR-arcs. This source extends to higher altitudes than the sources used by Walker, et. al. (20), Breig et. al., (22) and Schunk and Hays (23). As a result, the molecular excitation occurs in a region of the thermosphere where vibrational energy exchange is slow in comparison with the diffusion process. Thus, because the source is non-Boltzmann in its energy distribution and because the excited molecules diffuse to lower altitudes where vibrational energy exchange is the dominant process, the assumptions of a Boltzmann distribution and negligible diffusion loss are no longer tenable. This work differs from that of Walker, et. al., (20) and Breig, et. al. (22), by not assuming a Boltzmann distribution, and from that of Schunk and Hays (23) by including diffusion of the excited molecules.

2.3 The equations of continuity.

The continuity equation for each energy level of vibrationally excited molecular nitrogen, N_2^* , governs the level population and its altitudinal distribution. For the ith level the equation is

$$\frac{\partial}{\partial t} n_i + \nabla \cdot (n_i \vec{v}_i) = Q_i - L_i \qquad (2\text{-}1)$$

where n_i is the number density of molecular nitrogen in energy level i

$\vec{v}_i$ is the vector velocity of transport of n_i

Q_i is the production rate of n_i

L_i is the loss rate of n_i.

In principal the production and loss rate terms contain all sources and sinks for the ith level. However, we are interested in solutions of (2-1) corresponding to SAR-arc conditions where the electron temperature is unusually large. In addition we are interested in a process which, to first order, can be considered as an additional source to those ordinarily present in the thermosphere.

Figure 2-1 shows the rates of the dominant processes for equation (2-1). Also included in Figure 2-1, for comparison purposes, are the total vibrational quanta production rates between 120 and 300 km. calculated from the work of Walker et. al. (20) and Kummuler and Bortner (25) and shown as squares and circles, respectively. Shown as triangles in Figure 2-1 are the CO_2 quenching rates for vibrationally excited nitrogen at 120 km. taken from references (20), (22) and (25).

The atomic oxygen quenching curve shown in Figure 2-1 was calculated using the reaction rate of 3.5×10^{-15} $cm^3 sec^{-1}$, (21), and the atomic oxygen number density shown in Figure 1-2. The curve of atomic oxygen production of N_2^* (translational-vibrational energy enchange process) was calculated from the quenching curve using detailed balance considerations. These curves correspond to $1 \rightarrow 0$ and $0 \rightarrow 1$ transitions of N_2 respectively.

The vibrational energy exchange curve was calculated for the $0 \rightarrow 1$, $1 \rightarrow 0$ transitions using the exact resonance case of the Schwartz-Slawsky-Herzfeld,

(SSH), theory, (27) page 330, and the molecular nitrogen number density profile of Figure 1-2.

The rate for diffusion was calculated from the diffusion coefficient, D, and the density scale height, H, for molecular nitrogen by

$$\text{rate} = \frac{D}{H^2} \tag{2-2}$$

This rate may be regarded as the inverse of the time for a nitrogen molecule to diffuse to an altitude where there is an appreciably greater density (by a factor of e) of molecular nitrogen.

The electronic production curve was calculated using the reaction rates for inelastic collisions between thermal electrons and molecular nitrogen discussed in Appendix I and the electron and molecular nitrogen densities and electron temperatures in Figures 1-2 and 1-3, respectively. The electron temperature used is that for a 17.7 KR SAR-arc. For the calculation it was assumed that the vibrational temperature was zero.

From Figure 2-1 it is seen that the source of vibrational energy from thermal electrons, under the SAR-ARC condition, is larger over most of the altitude range of interest than the source of vibrational energy from ordinary ionospheric processes (20), (25). Because of the uncertainty in the yield of vibrational energy from O (^{1}D) quenching by molecular nitrogen (20), (25), and because the O (^{1}D) density during SAR-arcs is enhanced and its spatial distribution is complex, we have ignored this potential source term. Thus, the source term, Q_i, in equation (2-1) will only include production of vibrationally excited nitrogen by collisions between nitrogen molecules and thermal electrons (and only

coincidentally by atomic oxygen) and vibrational energy exchange between nitrogen molecules. These approximations should underestimate the source terms and hence the calculated temperatures would tend to be a lower bound for this reason.

The dominant loss processes for vibrationally excited molecular nitrogen at higher altitudes is electron quenching at altitudes above 400 km. (20, 25), and diffusion above 320 km. (see Figure 2-1). At low altitudes the dominant loss processes are quenching by atomic oxygen for altitudes between 120 and 300 km (Walker et. al., (20), found that quenching by other minor constituents in the lower thermosphere through translational-vibration energy exchange was negligible) and vibrational energy exchange with CO_2 (20), (22), at 120 km. Thus, the loss term, L_i, in equation (2-1) will include loss by electron and atomic oxygen quenching and vibrational energy exchange with molecular nitrogen. The vibrational energy loss by molecular nitrogen to carbon dioxide will be included through a lower boundary condition on the vibrational temperature for the following reasons. The abundance of carbon dioxide at 120 km is somewhat uncertain and depends on the altitude of the turbopause. The turbopause of the atmosphere is below 120 km altitude. Thus, in the altitude region of interest, carbon dioxide could be expected to approach diffusive equilibrium. Because of its relatively large mass, the density of carbon dioxide should decrease rapidly above 120 km. and increase rapidly below 120 km. altitude, thus creating a loss process significant only at the lower boundary.

The source and loss terms for equation (2-1) are therefore given by

$$Q_i = \sum_{j=0}{}' A_{ij}\, n_j + \sum_{j=0} P_{i,j;i-1,j+1}\, \nu_{j+1,i-1}\, n_{j+1}$$

$$+ \sum_{j=1} P_{i,j:i+1,j-1}\, \nu_{j-1,i+1}\, n_{j-1} + C_{i,i-1}\, \nu_{i-1,[0]}\, n_{i-1} \qquad (2\text{-}3)$$

$$+ C_{i,i+1}\, \nu_{i+1,[0]}\, n_{i+1}$$

$$L_i = \sum_{j=0}{}' A_{ji}\, n_i + \sum_{j=0} P_{i-1,j+1:i,j}\, \nu_{ij}\, n_i$$

$$+ \sum_{j=1} P_{i+1,j-1:i,j}\, \nu_{ij}\, n_i \qquad (2\text{-}4)$$

$$+ C_{i-1,i}\, \nu_{i,[0]} + C_{i+1,i}\, \nu_{i,[0]}\, n_i$$

where a prime on the summation excludes j = i, and

$P_{i,j:i-1,j+1}$ is the exchange transition probability for a nitrogen molecule in level i - 1 going to level i while the collisional partner molecule goes from level j + 1 to level j.

$\nu_{i,j}$ is the collision frequency of a nitrogen molecule in level j with a molecule in level i.

$C_{i,j}$ is the probability for collisional transitions from level j to level i where the collision is with atomic oxygen atoms.

A_{ij} is the reaction rate, from Appendix I, for the transition from level j to level i due to collisions between thermal electrons and molecular nitrogen molecules in level j.

$\nu_{i,[0]}$ is the collision frequency of a molecule in level i with an atomic oxygen atom.

2.4 The coefficients in the equations of continuity.

The cross sections for the subexcitation, inealstic, scattering of electrons by molecular nitrogen (28), (29), (30) are only available for the first five energy levels. These cross-section calculations and the calculation of reaction rates from the cross-sections are discussed in Appendix 1.

We will assume that molecular nitrogen can be represented by a harmonic oscillator. Thus, only transitions between adjacent levels will be considered. This assumption is appropriate for the moderate vibrational temperatures of this problem where only the lower lying energy levels are important and where anharmonic effects are small (31), (32), (33). It is also implicit to this calculation that the first five excited levels of molecular nitrogen will be considered as the totality of excited levels.

The above assumption and the theory for exact resonance vibrational-vibrational energy exchange of SSH, (27), allow us to write the vibrational-vibrational energy exchange probability in terms of the $0 \rightarrow 1$, $1 \rightarrow 0$ transitions of molecular nitrogen as

$$P_{i,j:i-1,j+1} = i(j+1)\, P_{1,0:0,1} \tag{2-5}$$

From detailed balance considerations

$$P_{i-1,j+1:i,j} = P_{i,j:i-1,j+1} \tag{2-6}$$

Setting the steric factor in the SSH theory to three, and using the Lennard-Jones potential parameters for N_2 from table 66-1 of (27), and table 66-5 of (27) for the characteristic ℓ of the theory, we have

$$P_{i,j:i-1,j+1} = 2.600322 \times 10^{-6}\, i(j+1)\, T\, e^{91.5/T} \tag{2-7}$$

where T is the kinetic gas temperature.

It is assumed that

$$C_{i+1,i} = (i+1)\, C_{1,0} \tag{2-8}$$

for the translational-vibrational energy exchange probability, the reason will become apparent later. Thus, (2-8) is consistent with SSH theory,[3] but $C_{1,0}$ will not be determined from this theory (see reference (21)). Detailed balance gives

$$C_{i,i-1} = C_{i-1,i}\, e^{-\theta/T} \tag{2-9}$$

where θ is the characteristic temperature of N_2 ($\theta = 3380°K$).

We assume that the vibrational level in which the nitrogen molecule resides does not effect its collision cross section for both molecules and atoms. Thus we write

$$\nu_{ji} = \nu n_i \tag{2-10}$$

$$\nu_{i,[0]} = \nu' n[0], \tag{2-11}$$

Equations (2-3) and (2-4) become respectively

$$Q_i = \sum_{j=0} A_{ij}\, n_j + P_{1,0:0,1}\, \nu \sum_{j=0} i(j+1)\, n_{i-1}\, n_{j+1} + P_{1,0:0,1}\, \nu \sum_{j=1} j(i+1)\, n_{i+1}\, n_{j-1} + C_{1,0}\, \nu' n[0]\, [i\, n_{i-1} + (i+1)\, e^{\theta/T}\, n_{i+1}] \tag{2-12}$$

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[3] The measured reaction rate for $C_{0,1}$ is several orders of magnitude larger than would be calculated using SSH theory. The reason for the discrepancy may be that chemical interactions are responsible for the anomalous quenching, whereas SSH theory attributes the interaction as being due to short range repulsive potentials.

$$L_i = \sum_{j=0}' A_{ji}\, n_i + P_{1,0:0,1}\,\nu \sum_{j=0} i(j+1)\, n_i\, n_j + P_{1,0:0,1}\,\nu \sum_{j=i} j(i+1)\, n_j\, n_i + C_{1,0}\,\nu'\, n[0]\,[i\, e^{\theta/T} + (i+1)]\, n_i \tag{2-13}$$

The quantity ν in equations (2-10), (2-12) and (2-13) is calculated from equation (36-3) of reference (27)

$$\nu = \frac{1.271\, p}{\eta_{N_2}\, n} \tag{2-14}$$

where

p is the gas pressure

N_2 is the viscosity for molecular nitrogen

n is the total number density of molecular nitrogen

Using the ideal gas law, we have

$$\nu = \frac{1.271\, kT}{\eta_{N_2}} \tag{2-15}$$

where k is Boltzmann's constant. Using (8.2-18) of reference (34), and average values of the appropriate parameters for temperatures of 355°K and 1500°K, we obtain for ν

$$\nu = 1.482094 \times 10^{-11} \sqrt{T} \tag{2-16}$$

The quantity $C_{1,0}\,\nu'$ occurring in equations (2-12) and (2-13) is calculated from $C_{01}\,\nu'$ by equation (2-9), where $C_{01}\,\nu'$ is considered to be a "lumped" constant equal to the reaction rate constant reported by McNeal, et. al., (21) and is considered constant with altitude.

It will be assumed that the neutral atmosphere is static, and uniform horizontally in all of its parameters. The transport velocity, $\vec{v}_i$, is then the diffusion

velocity for molecular nitrogen through the atmosphere, and is given by (35), page 244,

$$\vec{v}_i = - D \left[\frac{1}{p_i} (\nabla p_i - \rho_i \vec{g}) + k_T \frac{1}{T} \nabla T\right] \tag{2-17}$$

where

D is the binary diffusion coefficient for molecular nitrogen, assumed to be independent of vibrational excitation.

p_i is the pressure of the molecular nitrogen in energy level i.

ρ_i is the mass density of molecular nitrogen

k_T is the thermal diffusion ratio

$\vec{g}$ is the acceleration of gravity.

Using the ideal gas law in (2-17) we have

$$\vec{v}_i = - D \left[\frac{1}{n_i} \nabla n_i + (k_T + 1) \frac{1}{T} \nabla T + \frac{mg}{kT} \hat{k}\right] \tag{2-18}$$

where $\hat{k}$ is a unit vector in the vertical direction

m is the mass of molecular nitrogen.

Rewriting (2-18) we have

$$\vec{v}_i = - D \left[\frac{1}{n_i} \nabla n_i + \frac{1}{H} \hat{k}\right] \tag{2-19}$$

where

$$\frac{1}{H} = (k_T + 1) \frac{1}{T} \frac{\partial T}{\partial z} + \frac{mg}{kT}, \tag{2-20}$$

and z is the vertical coordinate, positive upward and H is the density scale height. Thermal diffusion for molecular nitrogen is small, and therefore k_T will be set to zero. The flux term in equation (2-1) becomes

$$\vec{F}_i = n_i \vec{v}_i = - D \left[\nabla n_i + \frac{n_i}{H} \hat{k}\right] \tag{2-21}$$

It will be assumed that the magnetic field line is vertical, so that the SAR-arc is symmetrical about the vertical. Under this assumption the horizontal flux at the arc center vanishes. If, in addition, the divergence of the horizontal flux is ignored, equation (2-1) can be reduced to one spatial dimension corresponding to conditions at the arc center.

Under the above assumptions and using (2-21), (2-12) and (2-13), equation (2-1) becomes

$$\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial z}(\vec{F}_i)_z = \sum_{j=0} \{A_{ij} n_j - A_{ji} n_i\} + P_{1,0:0,1}\ \nu\, i \sum_{j=0} (j+1)\,[n_{i-1} n_{j+1} - n_i n_j] + P_{1,0:0,1}\,\nu\,(i+1) \sum_{j=1} j\,[n_{i+1} n_{j-1} - n_i n_j] + C_{1,0}\,\nu'\, n[0]\,[i\, n_{i-1} + (i+1) e^{\theta/T} n_{i+1} - (i\, e^{\theta/T} + i + 1)\, n_i] \tag{2-22}$$

2.5 Boundary conditions.

Two sets of boundary conditions will be used for equation (2-22).

For the first set we have

Initial condition: $n_i\ (z, 0) = 0$ for all $i > 0$

$= n$ for $i = 0$

Lower boundary: $n_i\ (120, t) = 0$ for all $i > 0$

$= n\ (120)$ for $i = 0$

Upper Boundary:

$$\left.\frac{\partial n_i}{\partial z}\right|_{z=\infty} = -\frac{n_i\ (\infty, t)}{H} \quad \text{for all } i.$$

The initial and lower boundary conditions correspond to all molecular nitrogen being in the ground state. This would correspond to total quenching by CO_2 at the lower boundary, and no excitation initially. The upper boundary condition insures zero flux, for all excited levels, at the top of the atmosphere.

For the second set of boundary conditions,

Initial Condition $\quad n_i(z, 0) = \dfrac{n}{1 - e^{-\theta/355}}\, e^{-i\,\theta/355} \quad$ for all i

Lower Boundary $\quad n_i\ (120, t) = \dfrac{n}{1 - e^{-\theta/355}}\, e^{-i\,\theta/355} \quad$ for all i

Upper boundary $\quad \left.\dfrac{\partial n_i}{\partial z}\right|_{z=\infty} = -\dfrac{n_i(\infty, t)}{H} \quad$ for all i

The initial and lower boundary conditions in this case correspond to assuming the vibrationally excited nitrogen to be Boltzmann distributed corresponding to a vibrational temperature of 355°K, the kinetic temperature at the lower boundary.

2.6 Simplification of equations and technique of solution.

In Appendix II the set of six, coupled, non-linear, partial differential equations (2-22) are replaced by seven equations in which the essential coupling is more

readily observed. This simplification is achieved by expressing the solutions of equation (2-22) as a sum of a Boltzmann distributed part and a part representing a deviation from a Boltzmann distribution, that is

$$n_i = n_i' + \epsilon_i \tag{A2-1}$$

It is then required that the Boltzmann distributed part, n_i', possess the total vibrational energy and number density of molecular nitrogen for the problem (see equations (A2-2) and (A2-3)). The deviation part, ϵ_i, is then a measure of the departure, at each altitude, of the solution from the energetically equivalent Boltzmann solution part. The differential equation to be solved for the Boltzmann part of the solution is

$$\frac{\partial \psi}{\partial t} - \frac{1}{n}\frac{\partial Dn}{\partial z}\frac{\partial \psi}{\partial z} - D\frac{\partial^2 \psi}{\partial z^2}$$

$$= \sum_{j=0} \sum_{i=0} \left[\frac{1}{\psi + 1}\left(\frac{\psi}{\psi + 1}\right)^j + \frac{\epsilon_j}{n}\right](i - j)\, A_{ij} \tag{A2-30}$$

$$+ C_{1,0}\, \nu' n[0] \left[\psi + 1 - e^{\theta/T}\psi\right]$$

where ψ is related to the partition function, Z_p, for the vibrationally excited nitrogen by

$$\psi = (Z_p - 1) \tag{A2-27}$$

The differential equation for the deviation part of the solution is

$$\frac{\partial}{\partial t}\varphi_i - D\frac{\partial^2}{\partial z^2}\varphi_i - \left[\frac{\partial D}{\partial z} + D\left(-\frac{1}{H} + 2\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right]\right.\frac{\partial \varphi_i}{\partial z}$$

$$+\left[\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z}\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\left\{\frac{\partial D}{\partial z} + D\left(-\frac{1}{H}\right.\right.\right.$$

$$\left.\left.\left.+\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right)\right\} - D\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial^2 \psi}{\partial z^2} - D\left(\frac{\partial \psi}{\partial z}\right)^2\left\{-\frac{i}{\psi^2}\right.\right.$$

$$\left.\left.+\frac{(i+1)}{(\psi+1)^2}\right\} + \sum_{j=0\ n} A_{ji}\,(1-\delta_{ij}) + P_{1,0:0,1}\,\nu n\,\{(2i+1)\,\psi + i\}\right.$$

$$\left.+ C_{1,0}\,\nu' n\,[0]\;(i\,e^{\theta/T} + i + 1)\right]\;\varphi_i = \sum_{j=0}\left\{A_{ij}\,(1+\varphi_j)\,e^{-(j-1)\theta/T_v}\right\}(1-\delta_{ij})$$

$$-\left[\left(\frac{i}{\psi} - \frac{i+1}{\psi+1}\right)\frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z}\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\left\{\frac{\partial D}{\partial z} + D\left\{-\frac{1}{H}\right.\right.\right.$$

$$\left.\left.+\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right\} + \sum_{j=0} A_{ji}\,(1-\delta_{ij}) - D\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial^2 \psi}{\partial z^2}\right.$$

$$- D\left(\frac{\partial \psi}{\partial z}\right)^2\left\{-\frac{i}{\psi^2} + \frac{i+1}{(\psi+1)^2}\right\} + P_{1,0:0,1}\,\nu n\,\{(2i+1)\,\psi + i\}$$

$$\left.+ C_{1,0}\,\nu' n\,[0]\;(i\,e^{\theta/T} + i + 1)\right] + P_{1,0:0,1}\,\nu n\,\{(2i+1)\,\psi + i\}$$

$$+ C_{1,0}\,\nu' n\,[0]\;\left[i\,e^{\theta/T_V} + (i+1)\,e^{\theta/T - \theta/T_V}\right] + \varphi_{i-1}\,e^{\theta/T_v}\left[P_{1,0:0,1}\,\nu n_i \gamma\right.$$

$$\left.+ C_{1,0}\,\nu' n\,[0]\;i\right] + \varphi_{i+1}\,e^{-\theta/T_V}\left[P_{1,0:0,1}\,\nu n(i+1)\,(\psi+1)\right.$$

$$\left.+ C_{1,0}\,\nu' n\,[0]\;e^{\theta/T}\,(i+1)\right] \qquad \text{(A2-46)}$$

where

$$\varphi_i = \frac{\epsilon_i}{n_i'} \tag{A2-39}$$

The boundary conditions are

set 1:

Initial condition $\psi(z, 0) = 0$

Lower boundary $\psi(120, t) = 0$

Upper boundary $\left.\frac{\partial \psi}{\partial z}\right|_{z=\infty} = 0$ (A2-31)

set 2:

Initial condition $\psi(z, 0) = 7.329241 \times 10^{-5}$

Lower boundary $\psi(120, t) = 7.329241 \times 10^{-5}$

Upper boundary $\left.\frac{\partial \psi}{\partial z}\right|_{z=\infty} = 0$ (A2-32)

set 1 and set 2

Initial condition $\varphi_i(z, 0) = 0$ for all i

Lower boundary $\varphi_i(120, t) = 0$ for all i

Upper boundary $\left.\frac{\partial \varphi_i}{\partial z}\right|_{z=0} = 0$ for all i (A2-47)

The set 1 boundary conditions on ψ correspond to a vibrational temperature initially zero, with the vibrational temperature at the lower boundary remaining zero, presumably due to quenching. The set 2 boundary conditions for ψ correspond to the initial vibrational temperature of 355°K (the kinetic temperature at the lower boundary) and the vibrational temperature at the lower boundary remaining at

355°K. In both cases the upper boundary condition on ψ corresponds to a zero flux of quanta through the top of the atmosphere.

The boundary conditions on the φ_i's correspond to zero deviations from a Boltzmann distribution initially, with zero deviation being maintained at the lower boundary (presumably due to the rapid vibration-vibration energy exchange among N_2 at this altitude).

Calculation shows that the source term for vibrational quanta due to electron collisions in equation (A2-30) is only mildly non-linear (less than 30%) for the electron and vibrational temperatures of interest here. It can also be argued, that for the relatively weak source of vibrational excitation for this problem, the departures from a Boltzmann solution will be such that the term ϵ_j/n will be small relative to 1. Thus by dropping the ϵ_j/n term in (A2-30), the ψ and φ_i equations are uncoupled, and a first approximation to ψ may be obtained by solving the equation

$$\frac{\partial \psi}{\partial t} - \frac{1}{n}\frac{\partial Dn}{\partial z}\frac{\partial \psi}{\partial z} - D\frac{\partial^2 \psi}{\partial z^2} = \sum_{j=0}\sum_{i=0}\left[\frac{1}{\psi+1}\left(\frac{\psi}{\psi+1}\right)^j\right](i-j)A_{ij}$$

$$+ C_{1,0}\,\nu' n[0]\,[\psi + 1 - e^{\theta/T}\psi] \qquad (2\text{-}23)$$

When ψ has been obtained, the vibrational temperature may be calculated by

$$T_v(z,t) = \frac{\theta}{\ln\left[\frac{\psi(z,t)+1}{\psi(z,t)}\right]} \qquad (2\text{-}24)$$

and the coefficients of equations (A2-46) are known functions of altitude and time. A first approximation to the φ_i's can then be obtained by solving equation (A2-46).

If necessary, a second approximation to ψ may be obtained from equation (A2-30) by using the first approximation of the φ_i's to determine ϵ_j/n in the source term of equation (A2-30) and resolving equation (A2-30). A second approximation to the φ_i's can then be obtained by using the second approximation for ψ in equations (A2-46). Higher approximations may in principle be found by repeating this process.

2.7 Finite difference equations and solutions.

In Appendix III it is shown that the finite difference equations for both equations (A2-30) and (A2-46) take the general forms

$$- A_\ell \psi_{\ell+1}^{m+1} + B_\ell \psi_\ell^{m+1} - A_\ell \psi_\ell^{m+1} = D_\ell^m \qquad \text{(A3-7)}$$

and

$$- {}^{\ell}A_i \, {}^{\ell+1}\varphi_i^{m+1} + {}^{\ell}B_i \, {}^{\ell}\varphi_i^{m+1} - {}^{\ell}A_i \, {}^{\ell-1}\varphi_i^{m+1} = {}^{\ell}C_i^m \qquad \text{(A3-17)}$$

where ℓ refers to an altitude grid point, with $\ell = 1$ the bottom boundary and $\ell = L$ the top boundary, m refers to a time grid point and i refers to the energy level being solved for. The boundary conditions become for ψ

	set 1	set 2
$m = 1$	$\psi_\ell^1 = 0$	$\psi_\ell^1 = 7.329241 \times 10^{-5}$
$\ell = 1$	$\psi_1^m = 0$	$\psi_1^m = \psi_\ell^1$
$\ell = L$	$\psi_L^m - \psi_{L-1}^m = 0$	$\psi_L^m - \psi_{L-1}^m = 0$

(A3-8) (A3-9)

and for the ϕ_i's

$$\begin{aligned} m = 1 \quad & {}^{\ell}\phi_i^1 = 0 && \text{for all } i \\ \ell = 1 \quad & {}^{1}\phi_i^m = 0 && \text{for all } i \\ \ell = L \quad & {}^{L}\phi_i^m - {}^{L-1}\phi_i^m = 0 && \text{for all } i \end{aligned} \tag{A3-18}$$

The two equations (A3-7) and (A3-17) are of the same form. We follow Richtmyer, (36), pages 103-104, for the solutions of (A3-7) and (A3-17). Only the solution of (A3-7) is presented here, because the extension to each of the equations in (A3-17) is clear.

It is seen that the right hand side of (A3-7) is a known quantity. Equation (A3-7) is a one parameter family, because any value of ψ_2^{m+1} determines a solution. Let

$$\psi_{\ell}^{m+1} = E_{\ell}\, \psi_{\ell+1}^{m+1} + F_{\ell} \tag{2-25}$$

which is also a one parameter family. We seek to find E_{ℓ} and F_{ℓ} such that the two families of solutions (2-25) and (A3-7) are the same. If (2-25) is to be true for any member of the family, the boundary conditions (A3-8) and (A3-9) require

$$E_1 = 0 \tag{2-26}$$

$$F_1 = \begin{cases} 0 & \text{set 1} \quad (2\text{-}27) \\ 7.329241 \times 10^{-5} & \text{set 2} \quad (2\text{-}28) \end{cases}$$

Substituting (2-25) into (A3-7) and placing the result in the form of (2-25) we have

$$\psi_{\ell}^{m+1} = \frac{A_{\ell}}{B_{\ell} - A_{\ell} E_{\ell-1}} \psi_{\ell+1}^{m+1} + \frac{D_{\ell}^{m} + A_{\ell} F_{\ell-1}}{B_{\ell} - A_{\ell} E_{\ell-1}} \tag{2-29}$$

Comparing equation (2-29) with (2-25) we have

$$E_{\ell} = \frac{A_{\ell}}{B_{\ell} - A_{\ell} E_{\ell-1}} \tag{2-30}$$

$$F_{\ell} = \frac{D_{\ell}^{m} + A_{\ell} F_{\ell-1}}{B_{\ell} - A_{\ell} E_{\ell-1}} \tag{2-31}$$

Using (2-26) and (2-27) or (2-28) we can calculate the $E\ell$'s and $F\ell$'s from $1 = 1$ to $1 = L$, that is, from the lower boundary to the upper boundary, by using (2-30) and (2-31), respectively.

When $1 = L - 1$, equation (2-25) gives

$$\psi_{L-1}^{m+1} = E_{L-1} \psi_{L}^{m+1} + F_{L-1} \tag{2-32}$$

Using the upper boundary condition of (A3-8) or (A3-9) in (2-32) we have

$$\psi_{L-1}^{m+1} = \frac{F_{L-1}}{1 - E_{L-1}} \tag{2-33}$$

We now repeat the process, for $\ell = L - 2, L - 3, \ldots, 1$, to solve for the ψ^{m+1}'s, that is, we solve for the ψ^{m+1}'s from the upper boundary to the lower boundary. This total process is repeated for each time step from $m = 1$ to the maximum time step of interest.

Only slight modification of this method is needed to solve for the six, coupled ϕ_i's of equation (A3-17).

The technique embodied in equations (A3-7) (A3-17) and equations (2-25) through (2-33) was programmed for the IBM 360-75 for both sets of finite difference equations (A3-7) and (A3-17). The program to solve for ψ was called BOLTSOL and the program to solve for the ϕ_i's was called BOLTDEV. Both programs are listed in Appendix IV. Details of the numerical solutions are discussed in Chapter III.

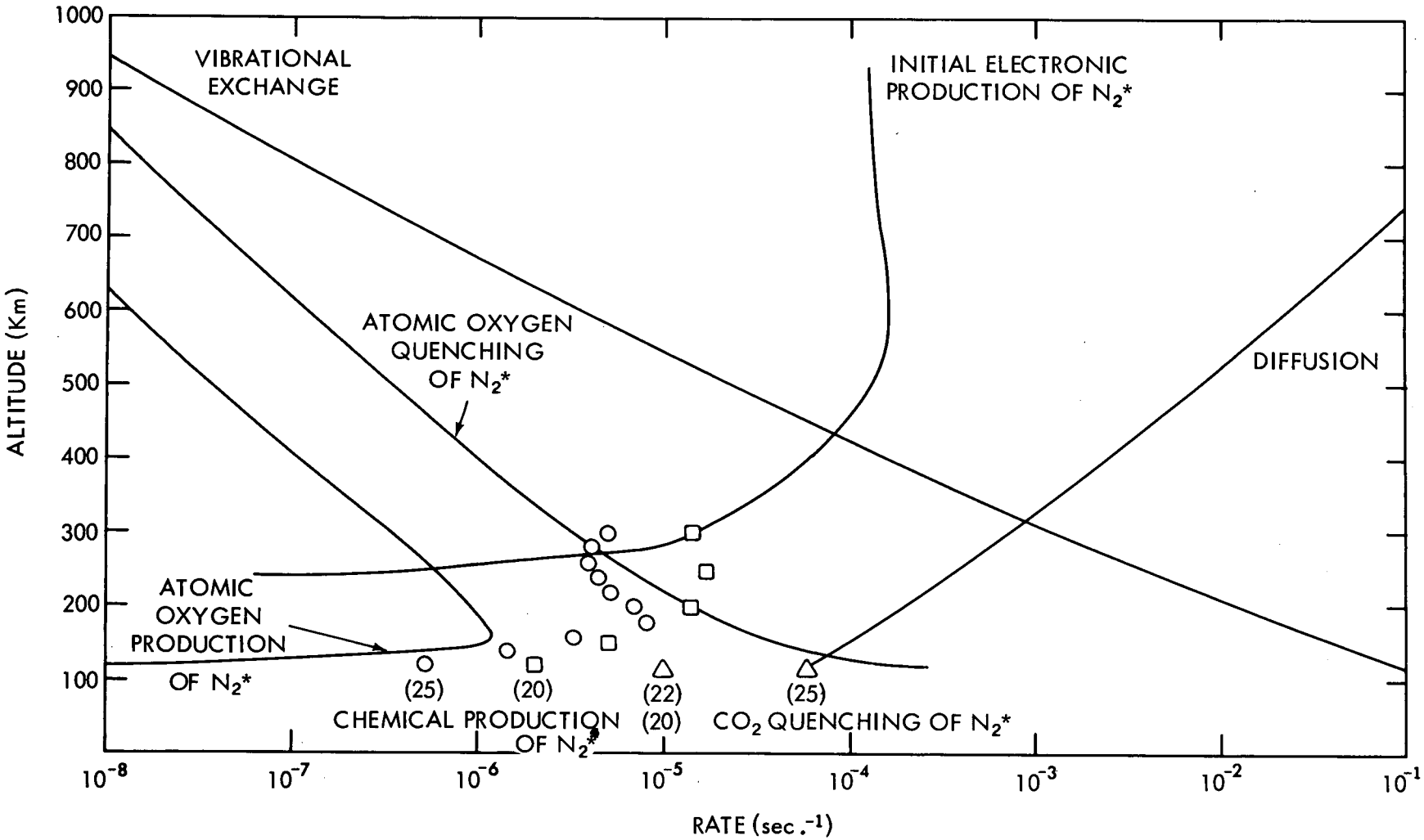

Figure 2-1. Rates of production and loss of vibrational energy and diffusion

CHAPTER III. APPLICATION TO SAR-arc

The finite difference equations (A3-7) and (A3-17) were solved in single precision over the altitude interval of 120 km to 920 km for conditions corresponding to those of a 17.7 KR SAR-arc, as shown in Figure 1-2 and 1-3. The upper altitude limit was lowered to 840 km. with negligible effect (less than 5° in the vibrational temperature and less than 2% in the ϕi's) on the solutions. The altitude step was taken as 40 km. and variation of the time step by a factor of 10, from 100 sec. to 10 sec. had no significant effect on the results. The solutions were generated over a time interval of 100000 seconds and approached (or reached) a steady state during that time.

Figure 3-1 shows the number of density of vibrational quanta versus altitude for a time into the solution of 95200 seconds. The number density of quanta was calculated from the solutions of equation (A3-7) corresponding to equation (2-23) (that is ignoring the ϵ_j/n term in the source term). Also shown in Figure 3-1 is the quantity $\sum_{i=0} i\,\epsilon_i$ calculated from the solutions of equations (A3-17). Theoretically equations (A2-4) and(A2-5) should be satisfied, however, because of the finite difference and other approximations, $\sum_{i=0} i\,\epsilon_i$ will not be zero. A measure of its significance is a comparison with the number of quanta calculated from the solutions of (A3-7). From Figure 3-1 it is seen that $\sum_{i=0} i\,\epsilon_i$ represents a negligible (<1%) portion of the energy in the Boltzmann solution for altitudes below 300 km. Between 300 and 600 km altitude, $\sum_{i=0} i\,\epsilon_i$ increases relative to the quantal number density, so that at altitudes of 600 km. and above $\sum_{i=0} i\,\epsilon_i$ represents only about 3% of the energy of the Boltzmann solution. These conclusions are valid at all other time steps.

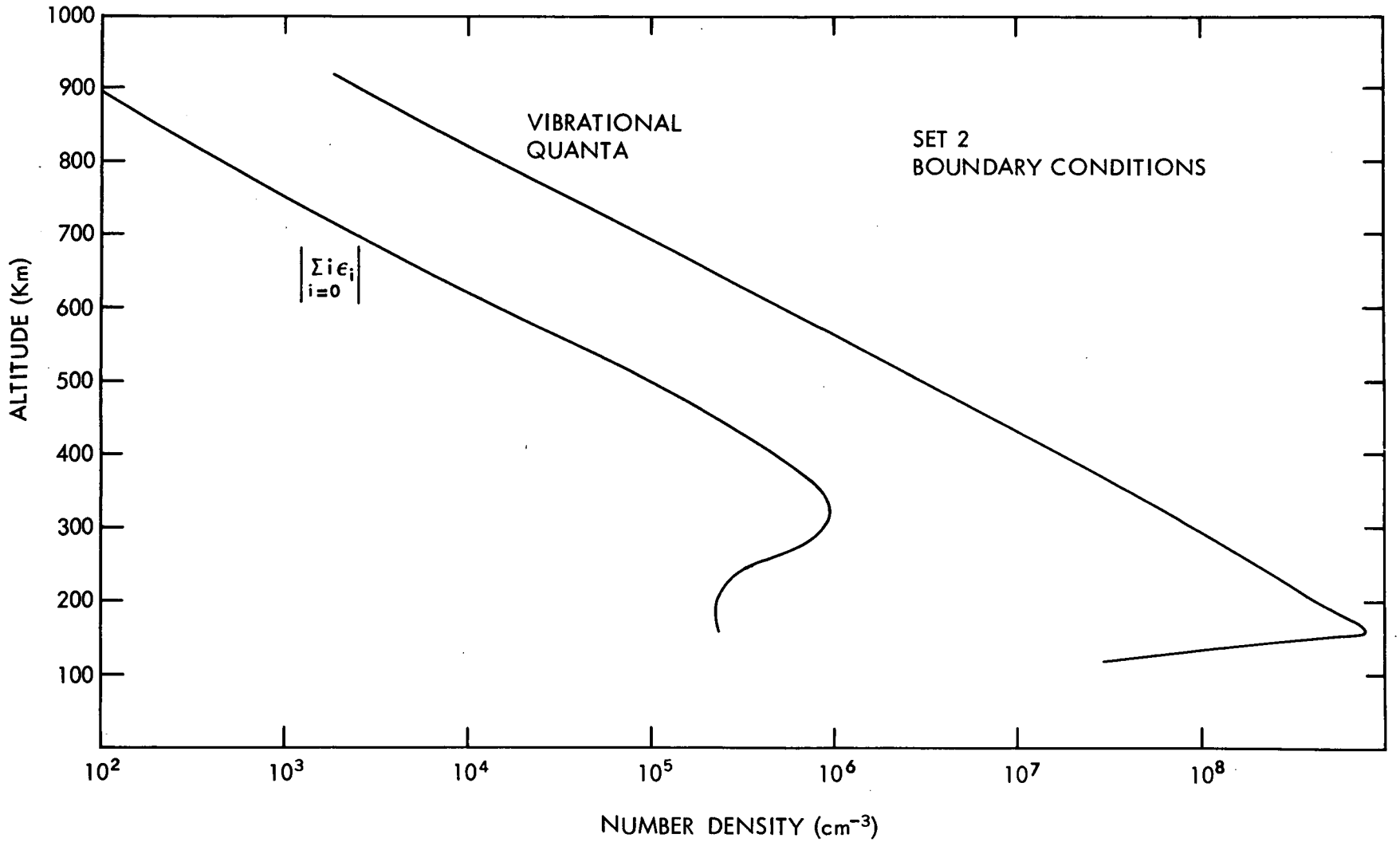

Figure 3-1. Comparsion of $\sum_{i=0} i\ \epsilon_i$ and the number density of vibrational quanta

Figure 3-2 is a plot of $\left|\sum_{i=0} \epsilon_i / \epsilon_i\right|$ versus altitude for each of the six energy levels corresponding to a time into the solution of 94700 seconds. This figure is also representative of the results at other times. It is seen in Figure 3-2 that below 400 km altitude $\sum_{i=0} \epsilon_i$ is comparable to or greater than the number densities of each of the deviations for all 6 energy levels. Above 400 km $\sum_{i=0} \epsilon_i$ is only several tens of percent of the deviations for levels 2 through 5 and a few percent of the deviations for levels 0 and 1. It should be pointed out that at 160 km. the ratio of the magnitudes of the deviations of level zero to level five (that is ϵ_0 / ϵ_5) is 10^7 initially, and for the time corresponding to Figure 3-2, is near 10^6. This explains why the ratios at 160 km. increase with level number. At 840 km. altitude, for the time corresponding to Figure 3-2, the ratio of ϵ_0 / ϵ_5 is near 10^2. It is significant that the ratio $\left|\sum_{i=0} \epsilon_i / \epsilon_i\right|$ has its largest values at the lowest altitudes where the deviations ϵ_i are numerically the largest. At low altitudes $\sum_{i=0} \epsilon_i$ is about 10^{-4} of the molecular nitrogen number density and at high altitudes it is about 10^{-3} of the molecular nitrogen number density. Figure 3-2 indicates that caution should be exercised in using the calculated deviations, ϵ_i, only for altitudes below 370 km. However, as later sections show, the influence of the deviations below 370 km. altitude is not large, but the ϵ_i do become physically important at higher altitudes where the precision of determination is considerably improved.

3.1 Solution for the Boltzmann part.

The vibrational temperatures calculated from the solution of the ψ equation are shown versus altitude and time in Figures 3-3 and 3-4, respectively. The solutions are for the set 2 (initial and lower boundary vibrational temperature of 355°K) boundary conditions.

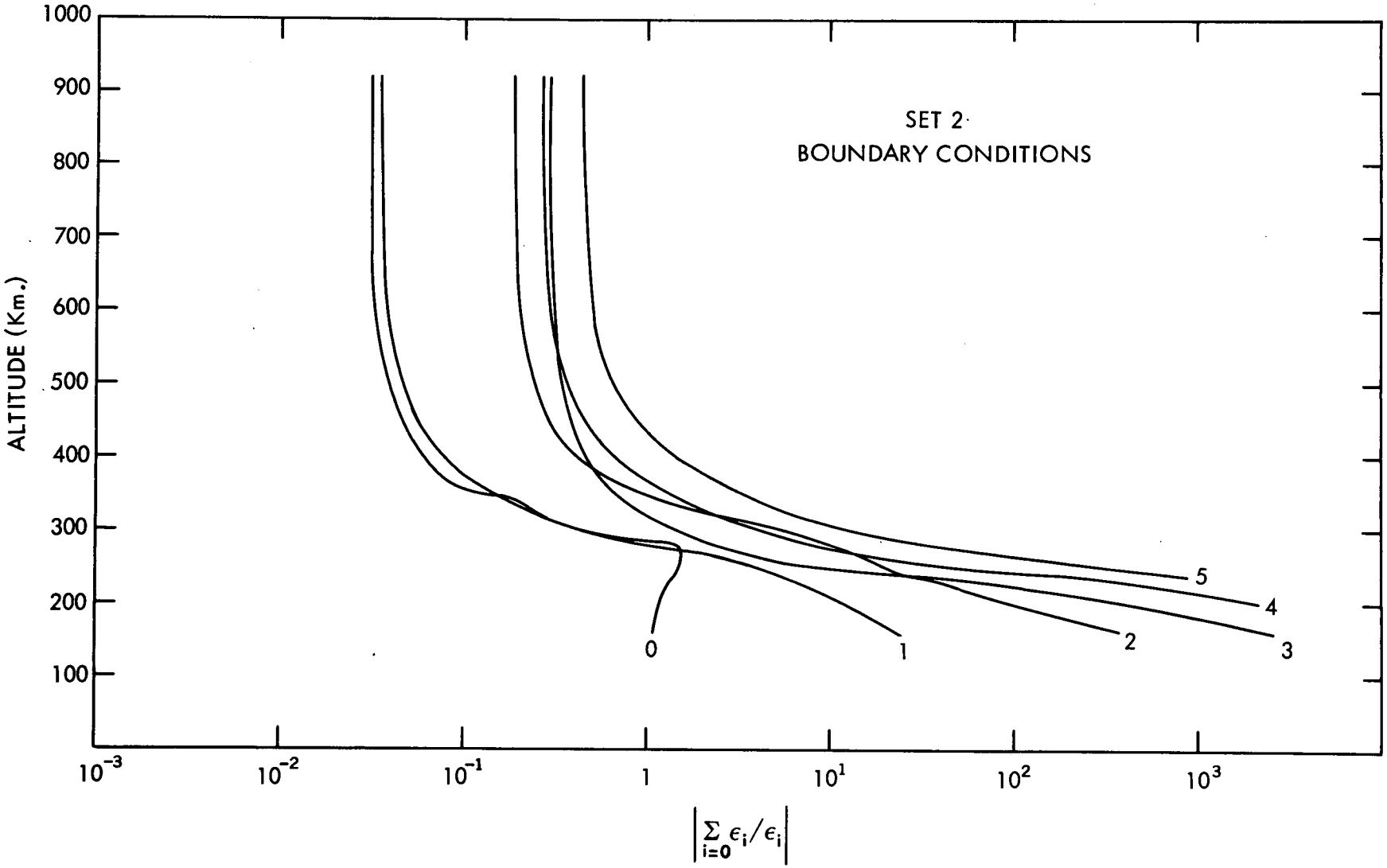

Figure 3-2. $\sum_{i=0} \epsilon_i/\epsilon_i$ for energy levels 0 through 5

Figure 3-3 shows the vibrational temperature profiles, calculated at five time steps, versus altitude. It is seen from this figure that at altitudes above 600 km the vibrational temperature is nearly isothermal at each time step, a result of the rapidity of the diffusion process at these altitudes. The downward movement of the energy is apparent in the figure. Vertical vibrational temperature gradients of as much as 25°K/km. are observed in the steady state.

Figure 3-4 is a plot of vibrational temperature versus time at ten altitudes of interest. It is seen from the figure that a steady state is reached in about one day. However, in 10 hours, or less depending on altitude, the vibrational temperature has achieved 90% or more of the steady state value. Notice that the vibrational temperature at the higher altitudes has a very steep gradient with time, initially. This rapid heating rate is important to the solutions of the deviation equations discussed in the next section. It should be noticed that the temperature at 240 km altitude has reached 1350°K, a value large enough to significantly effect the reaction constant of reaction (1-1), as discussed in section 3.3.

3.2 Solutions for the deviation parts.

It was found that convergence of the deviation solutions could not be achieved, even with 1 second time steps, if the solution was started at the "turn on" of the SAR-arc. It was determined that the difficulty was caused by terms involving derivatives of ψ and was apparently due to the initially very large changes in ψ primarily, those with time. Convergence of the solutions of the ϕ_i equations was obtained if the solutions were started at 5200 seconds "into" the arc, and this was the approach adopted. The physical conditions corresponding to the initial stages of a SAR-arc are unknown. However, it is expected that the characteristic times

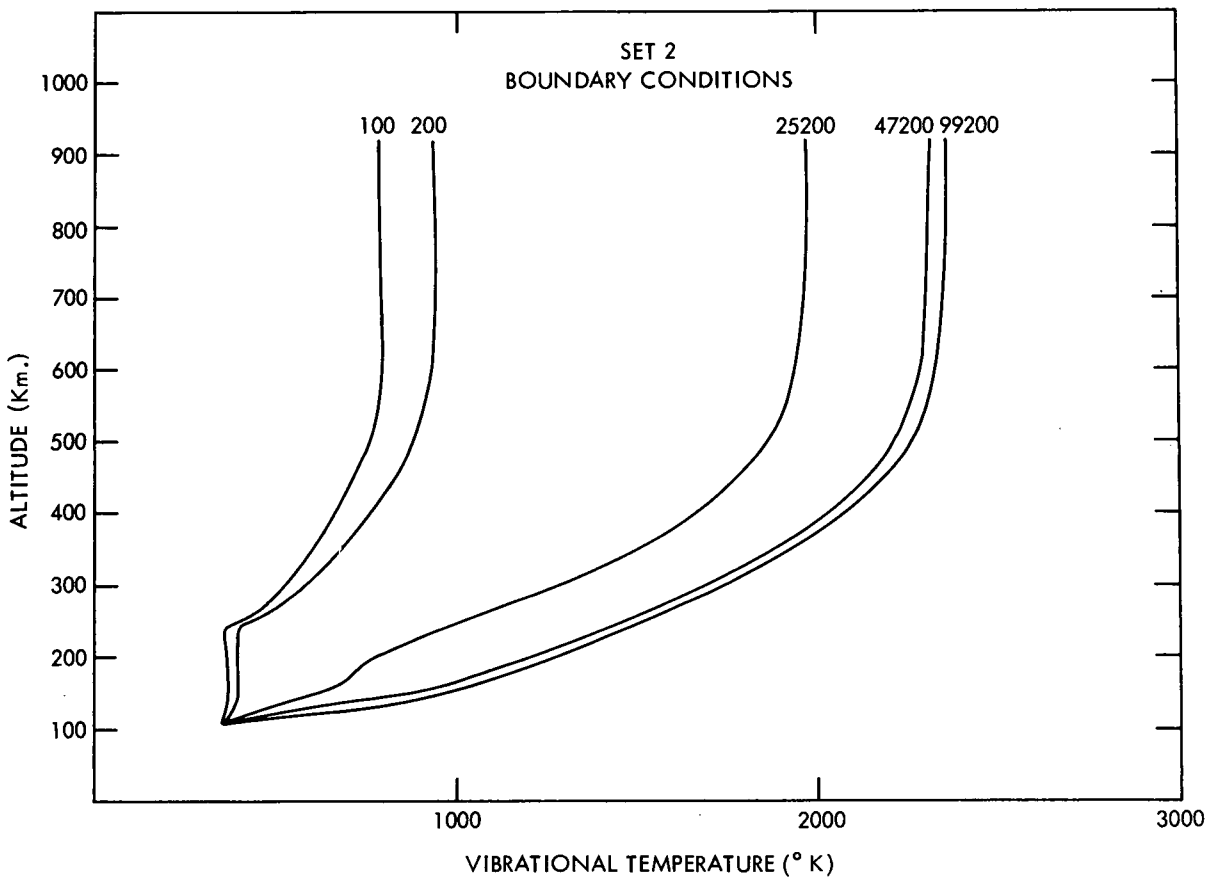

Figure 3-3. Vibrational temperatures calculated from the ψ equation solutions versus altitude for five time steps

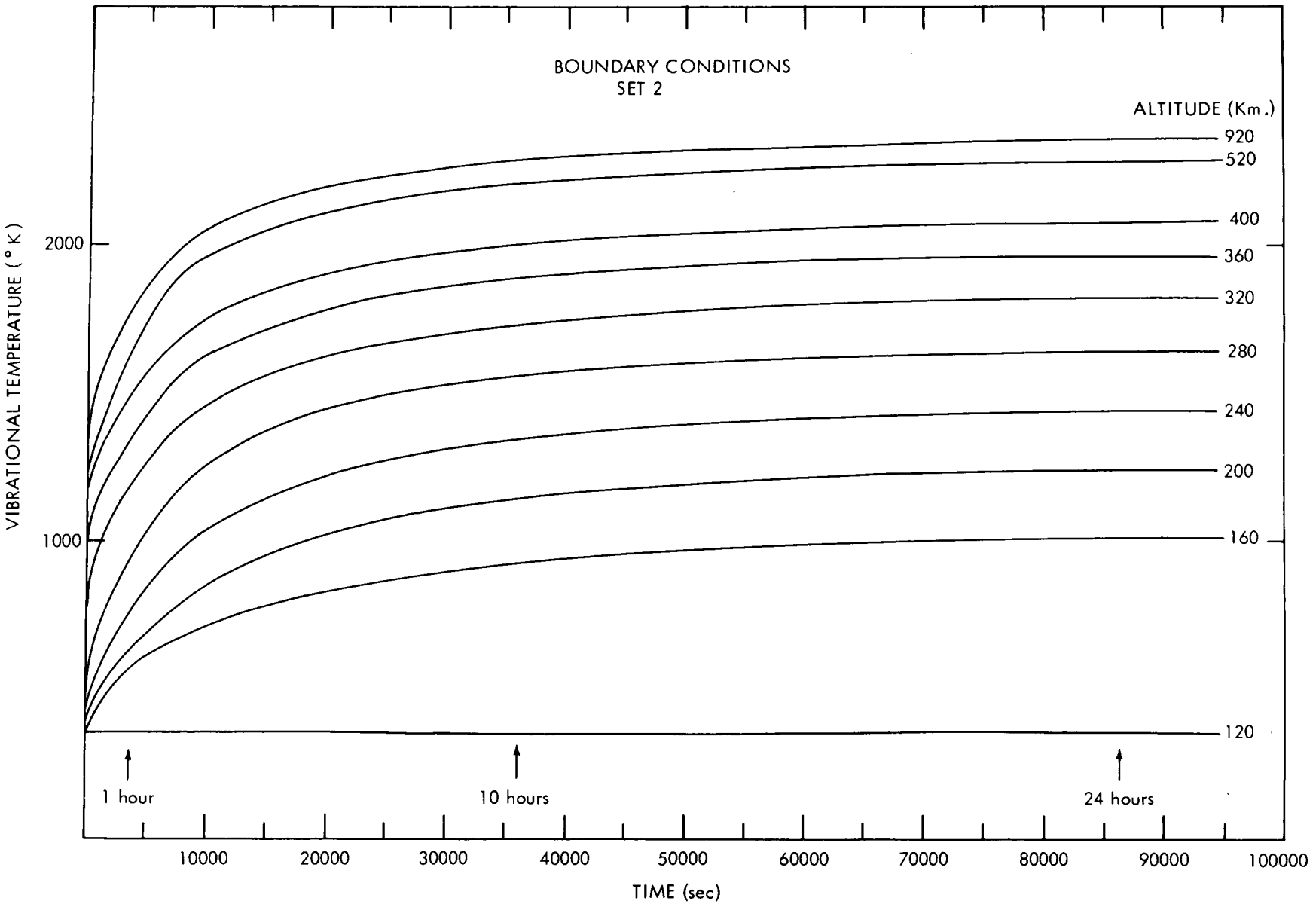

Figure 3-4. Vibrational temperatures calculated from the ψ equation versus time for several altitudes

of the important processes are measured in terms of one or more hours. Thus, the imposition of SAR-arc conditions in a step-wise manner is not realistic; so that little physical content has been lost by the adopted calculational approach.

Figures 3-5 through 3-10 show the ϕ_i's versus altitude for three time steps. These figures show that above 500 km the ratio of the deviation from the Boltzmann solution to the Boltzmann population, at the energy level of interest, is nearly constant with altitude. This result is again due to the rapidity of the diffusion process at these altitudes. It is also apparent from these figures that at altitudes of 300 km and above the ϕ_i's rapidly reach a maximum and then decrease to their "steady state" values. In these figures, where ϕ_i changes sign with altitude the absolute value has been plotted. It is seen that the "steady state" deviation populations above 300 km altitude, are less than the Boltzmann population of the corresponding energy levels 0, 1, 2 and 3 and are greater than the Boltzmann population for levels 4 and 5. This will be important in the calculation of an effective reaction coefficient for reaction (1-1) (see section 3.3).

Figures 3-11 through 3-16 show the ϕ_i 's versus times for several altitudes. From these figures it is seen that above 300 km altitude a nearly constant, significant, deviation is maintained from a Boltzmann distributed population for the upper energy levels.

3.3 Reaction rate constant for reaction (1-1) and ionospheric loss time constant.

The effective reaction rate constant for the ion-atom interchange reaction (1-1) was calculated from

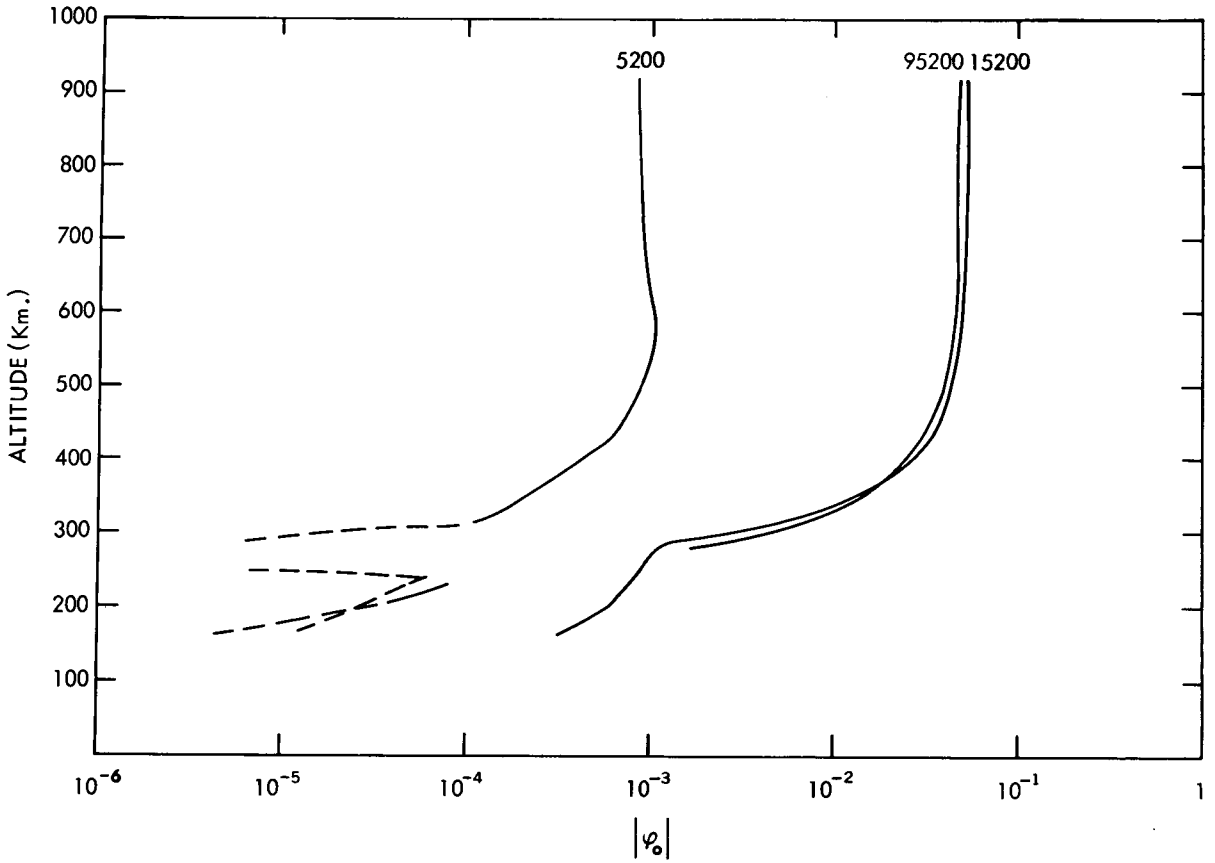

Figure 3-5. $|\phi_0|$ versus altitude for 3 time steps

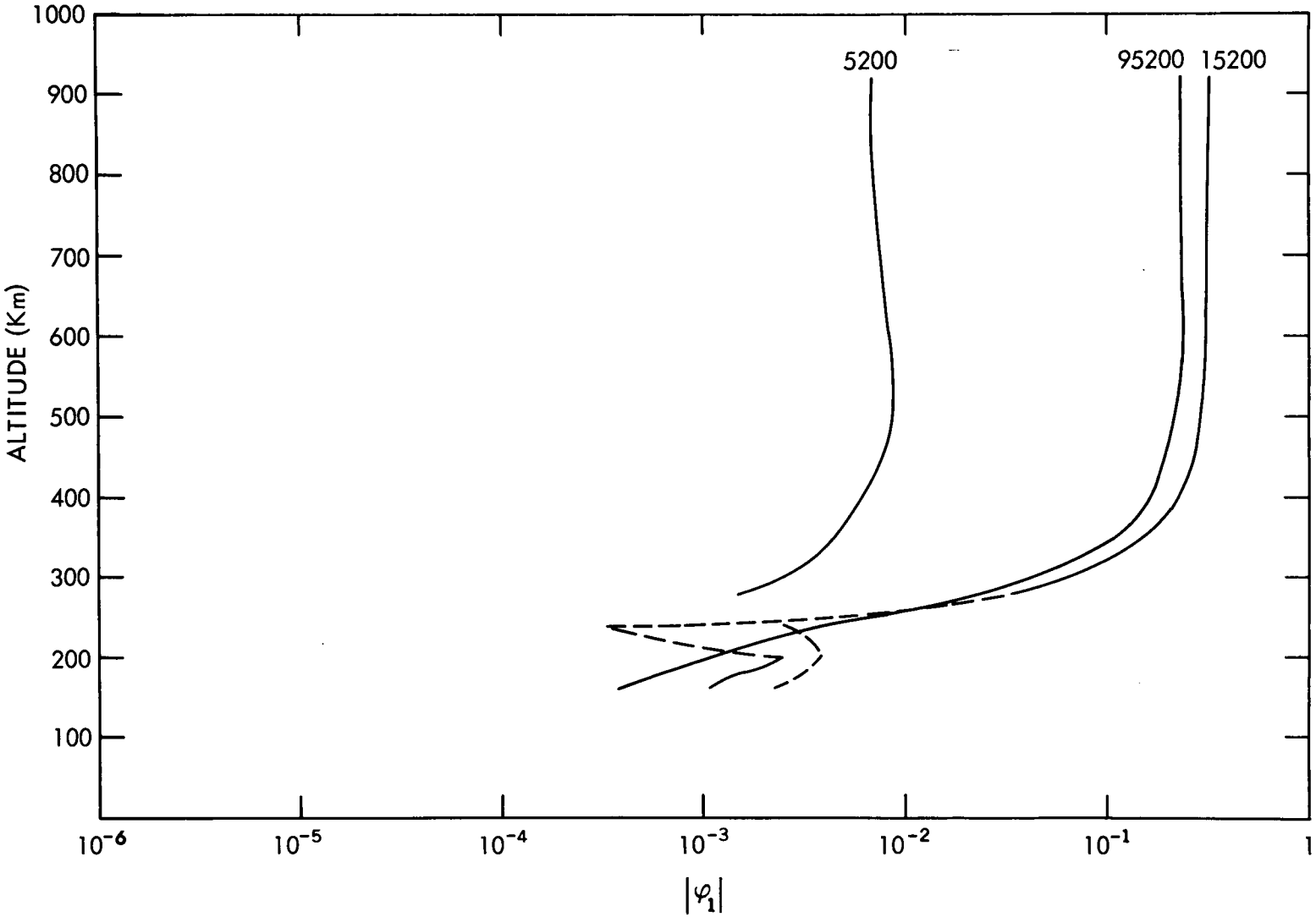

Figure 3-6. $|\phi_1|$ versus altitude for 3 time steps

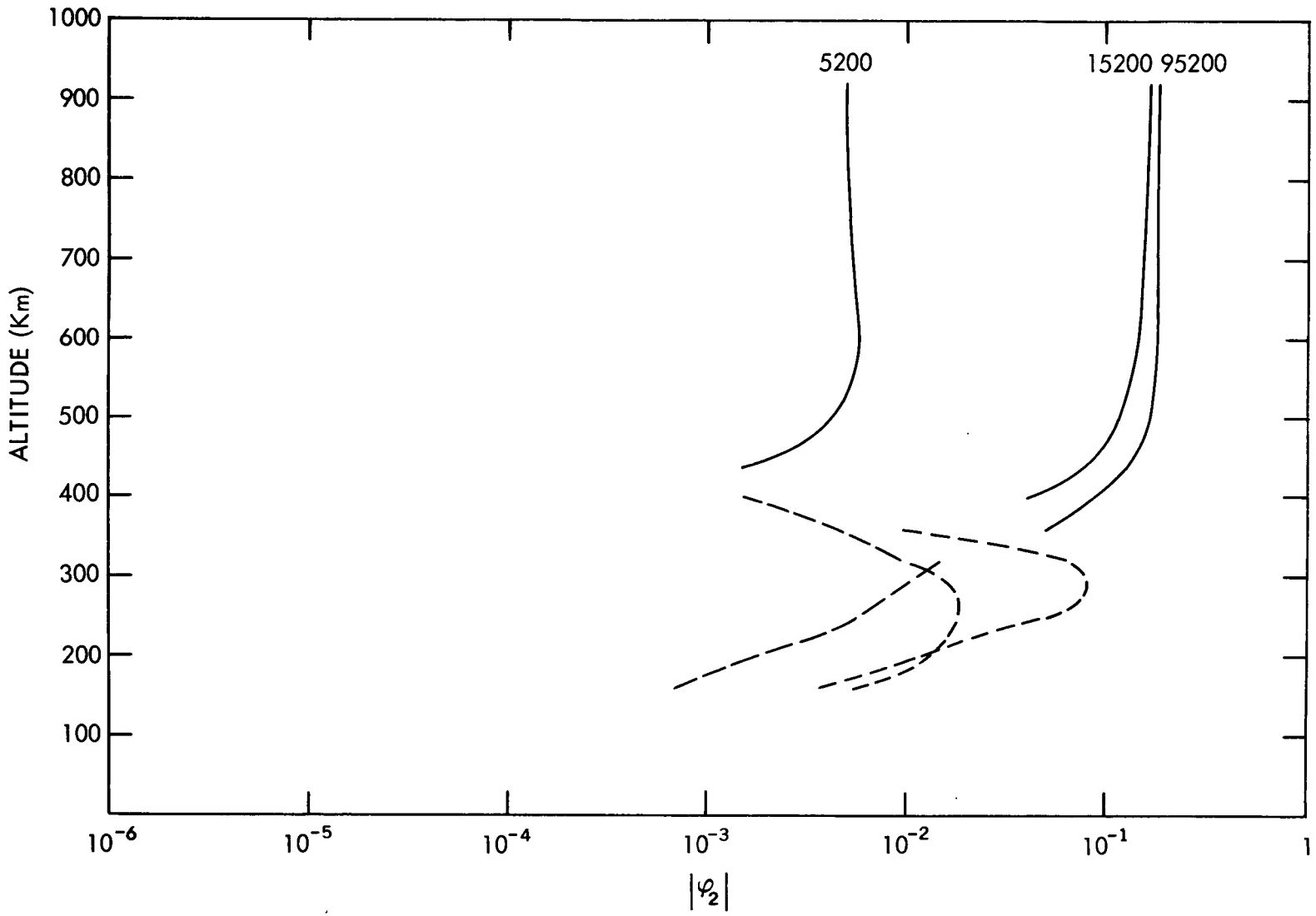

Figure 3-7. $|\phi_2|$ versus altitude for 3 time steps

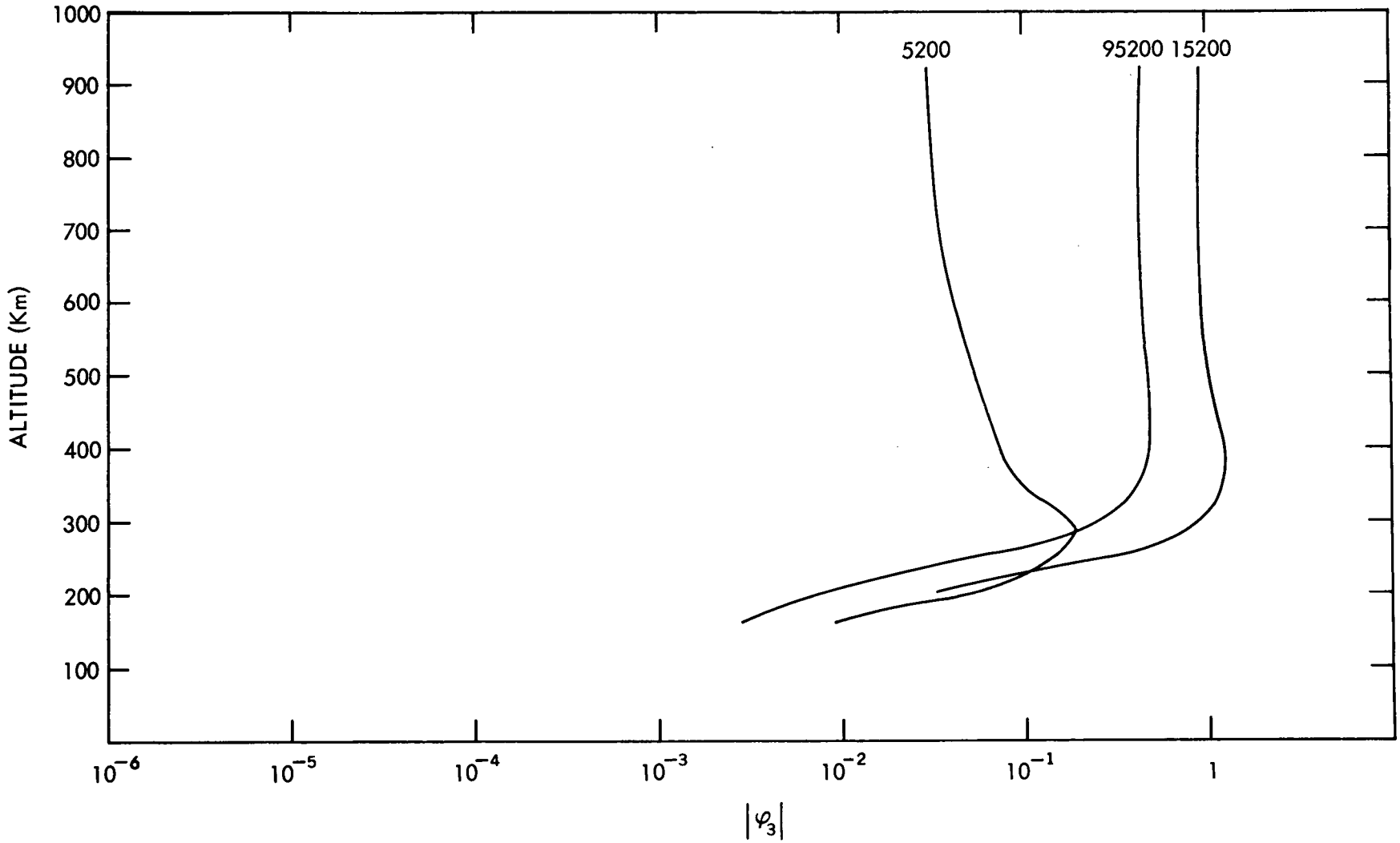

Figure 3-8. $|\phi_3|$ versus altitude for 3 time steps

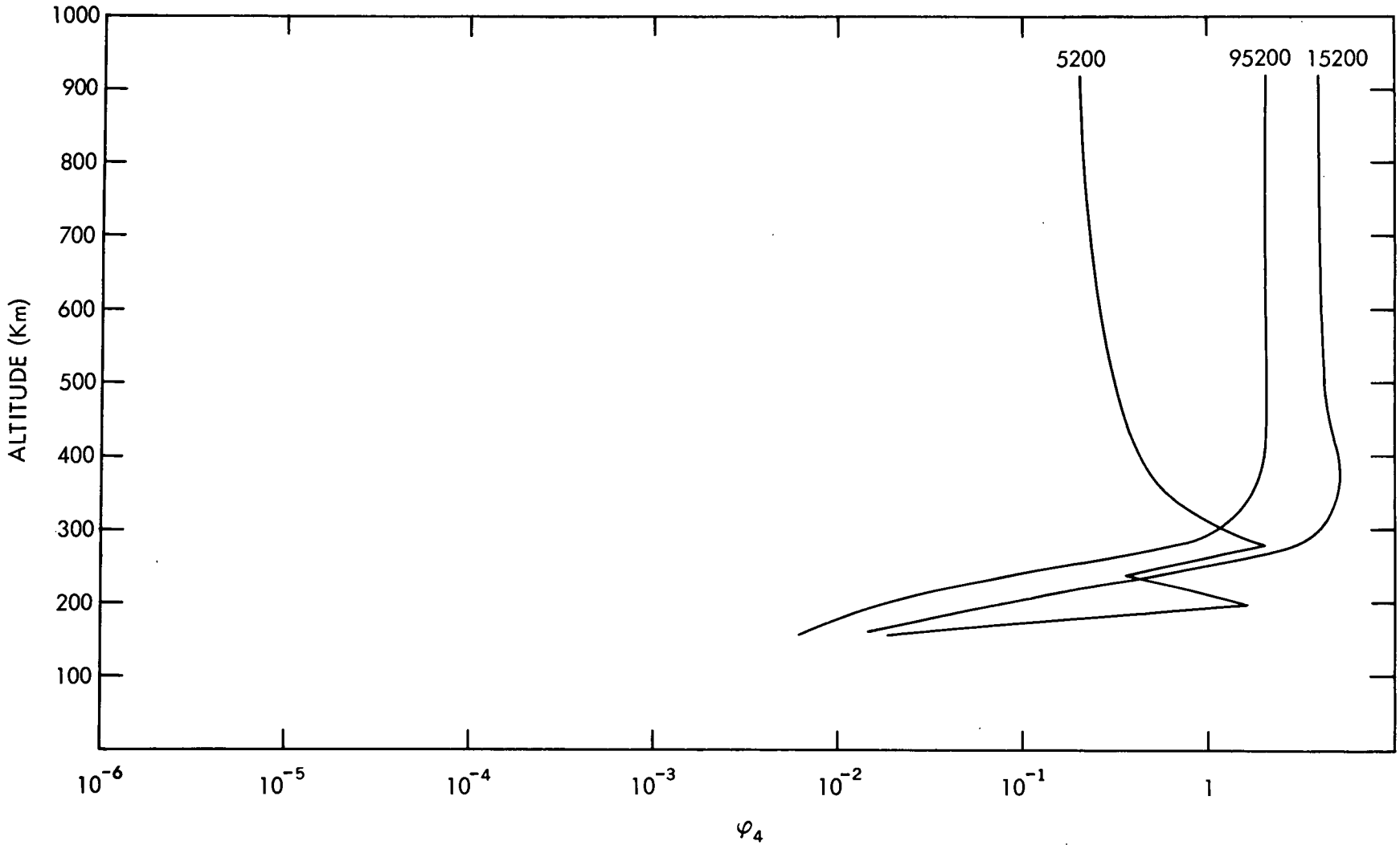

Figure 3-9. ϕ_4 versus altitude for 3 time steps

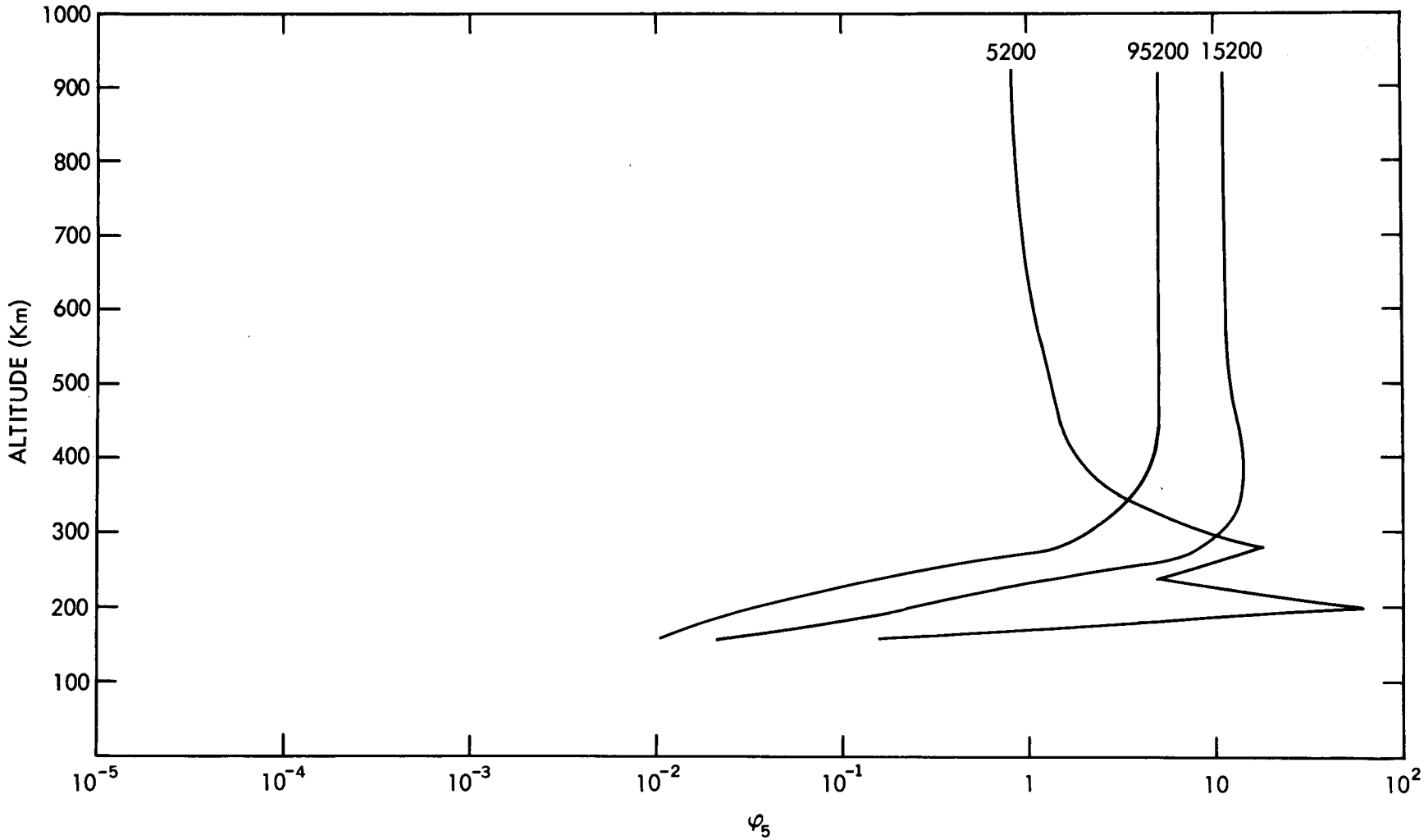

Figure 3-10. ϕ_5 versus altitude for 3 time steps

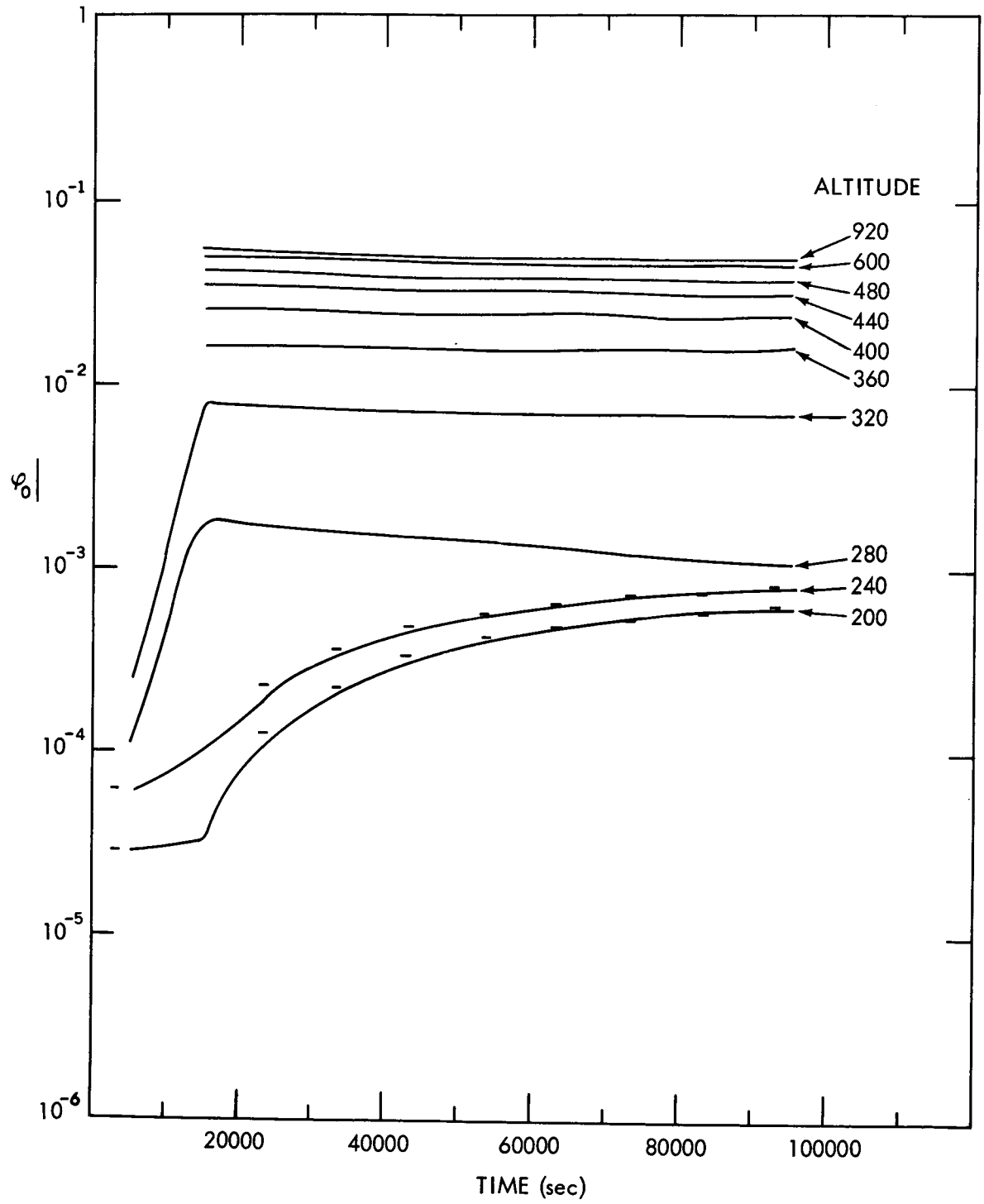

Figure 3-11. $|\phi_0|$ versus time for several altitudes

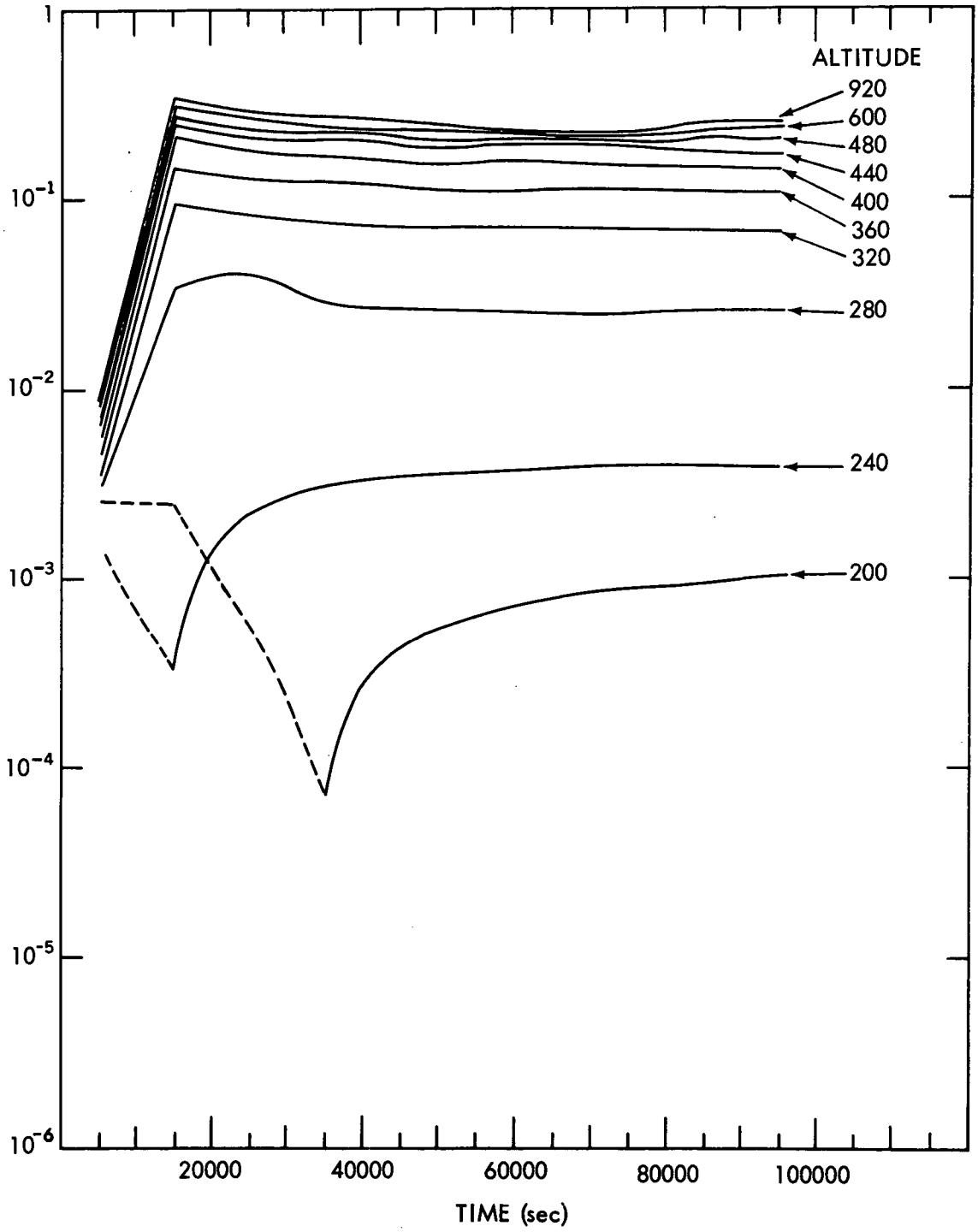

Figure 3-12. $|\phi_1|$ versus time for several altitudes

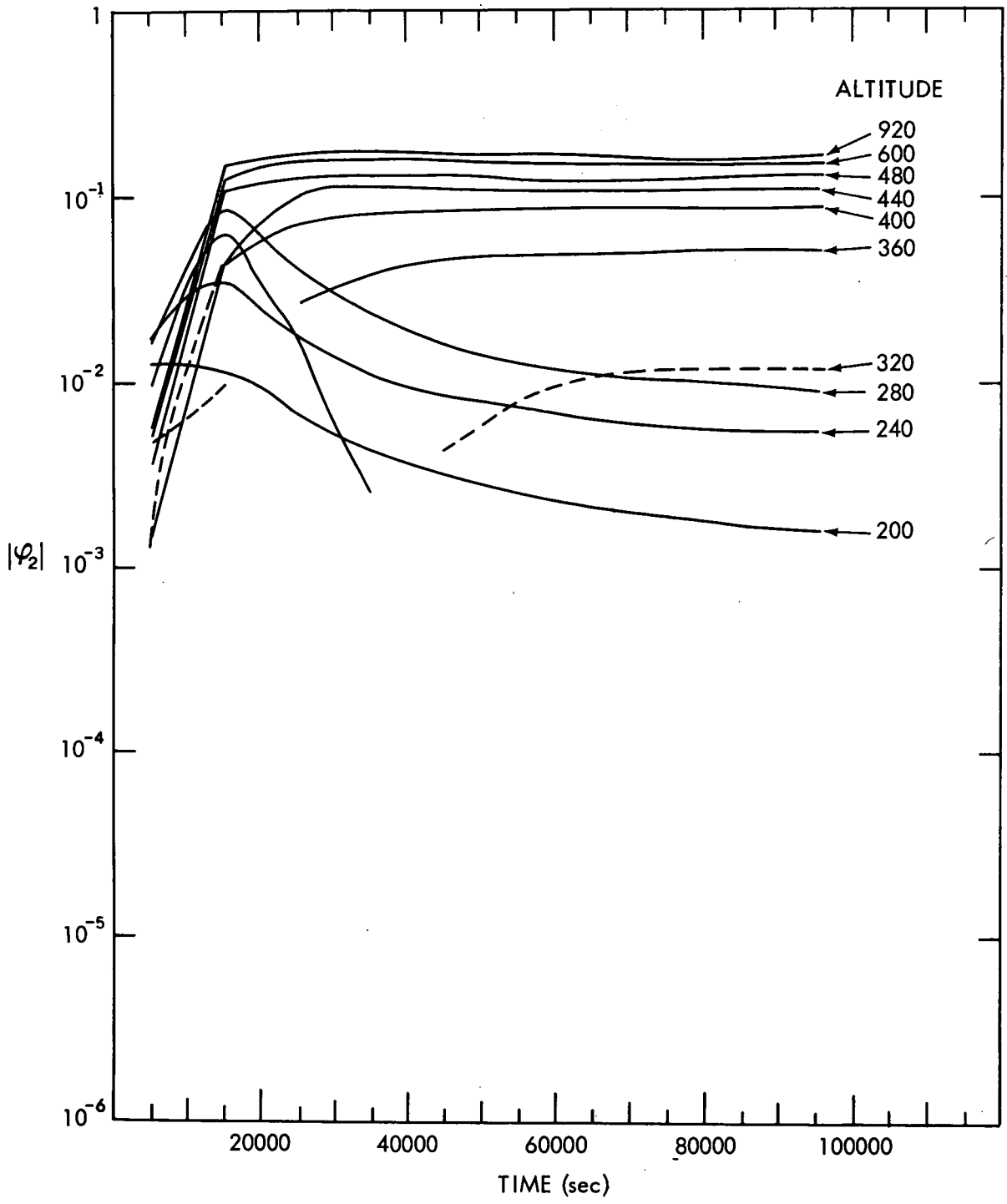

Figure 3-13. $|\phi_2|$ versus time for several altitudes

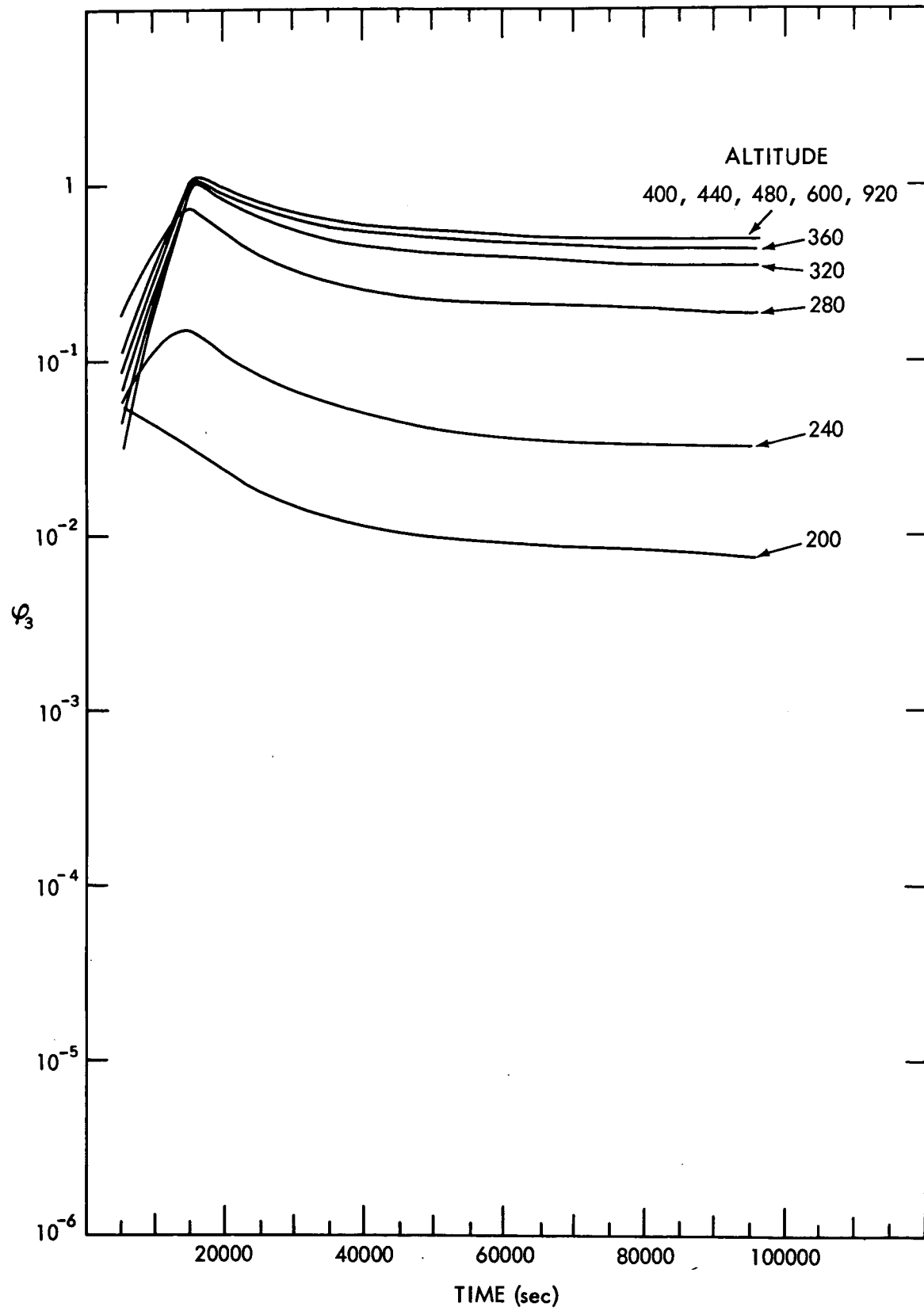

Figure 3-14. $|\phi_3|$ versus time for several altitudes

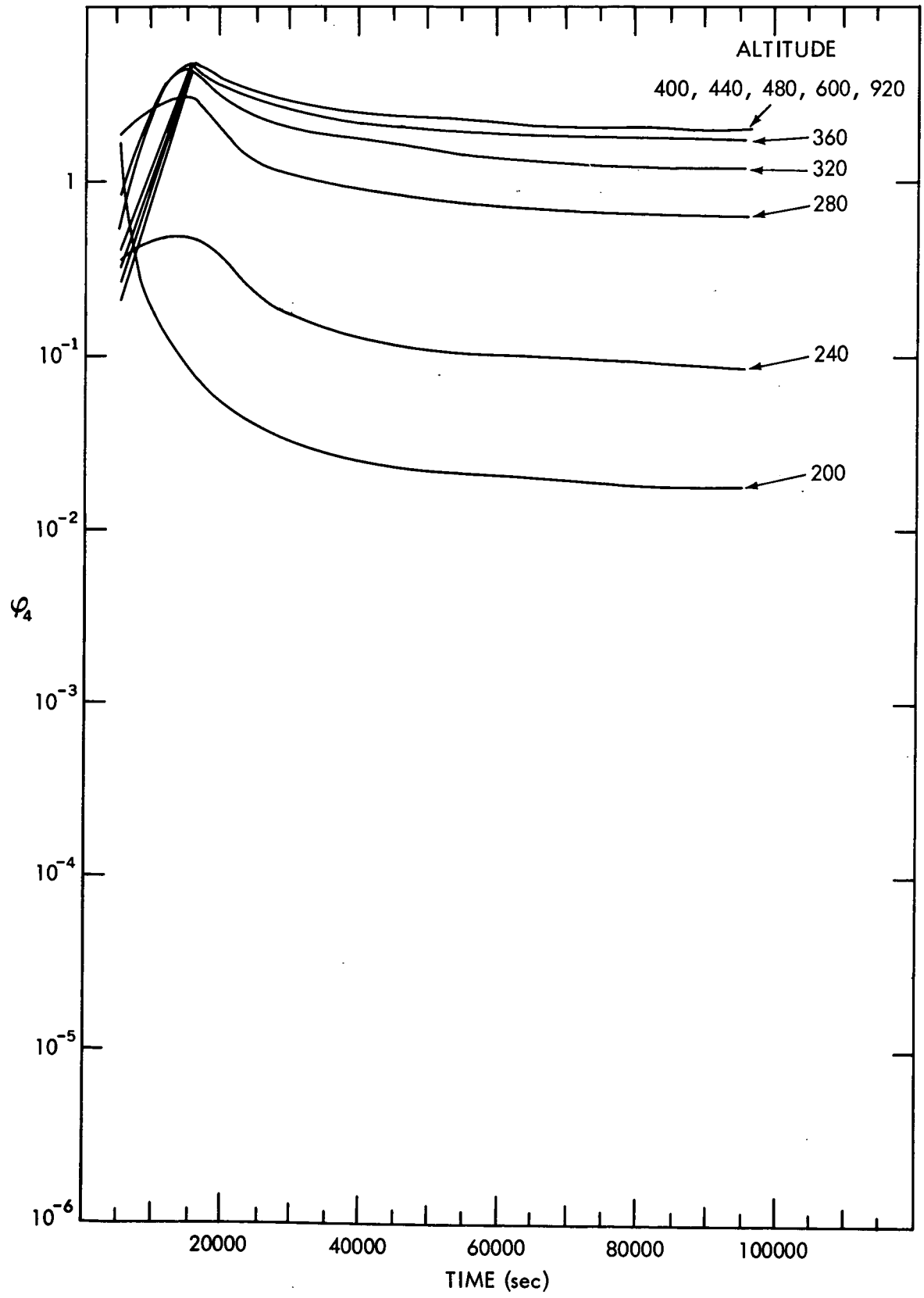

Figure 3-15. ϕ_4 versus time for several altitudes

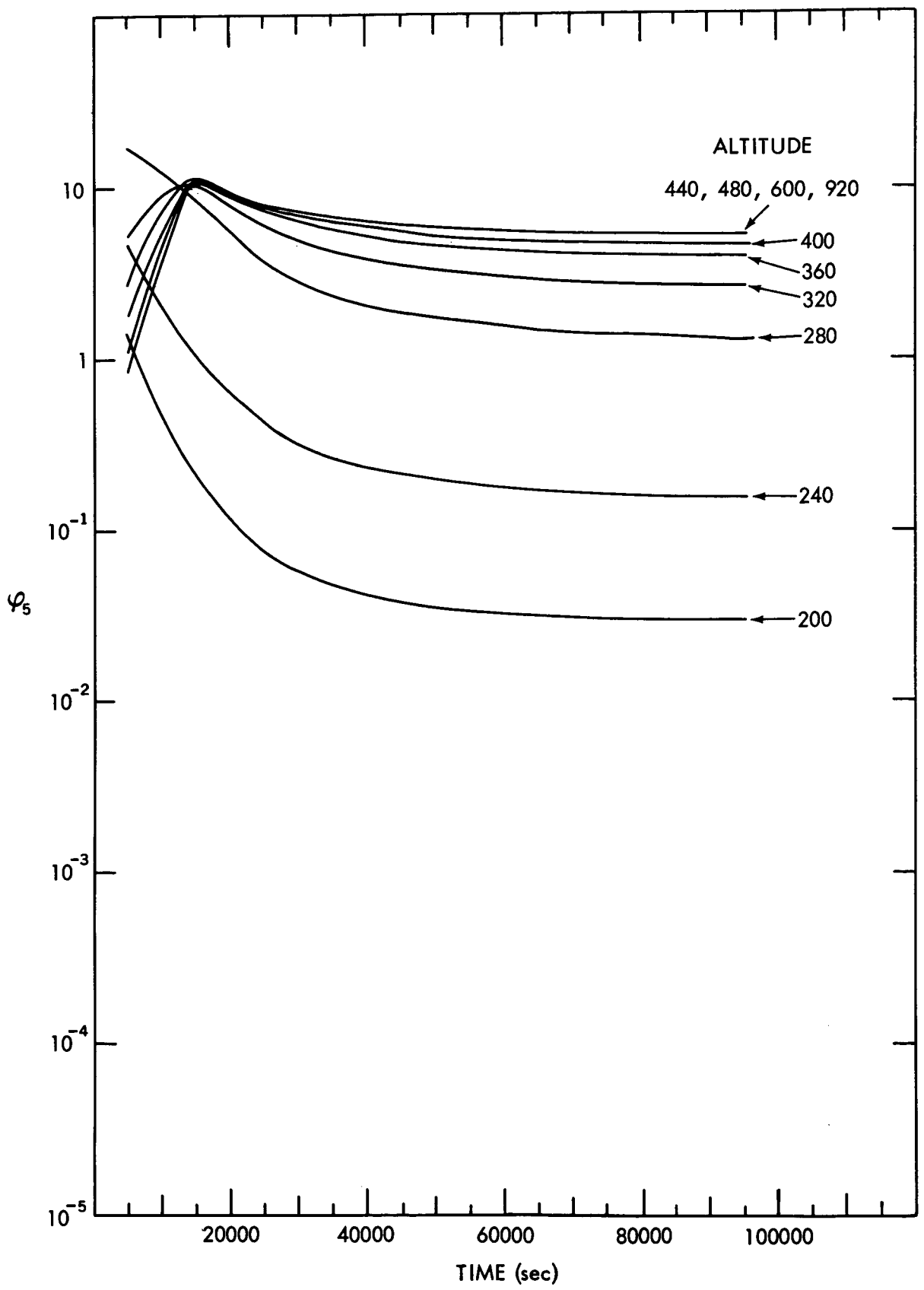

Figure 3-16. ϕ_5 versus time for several altitudes

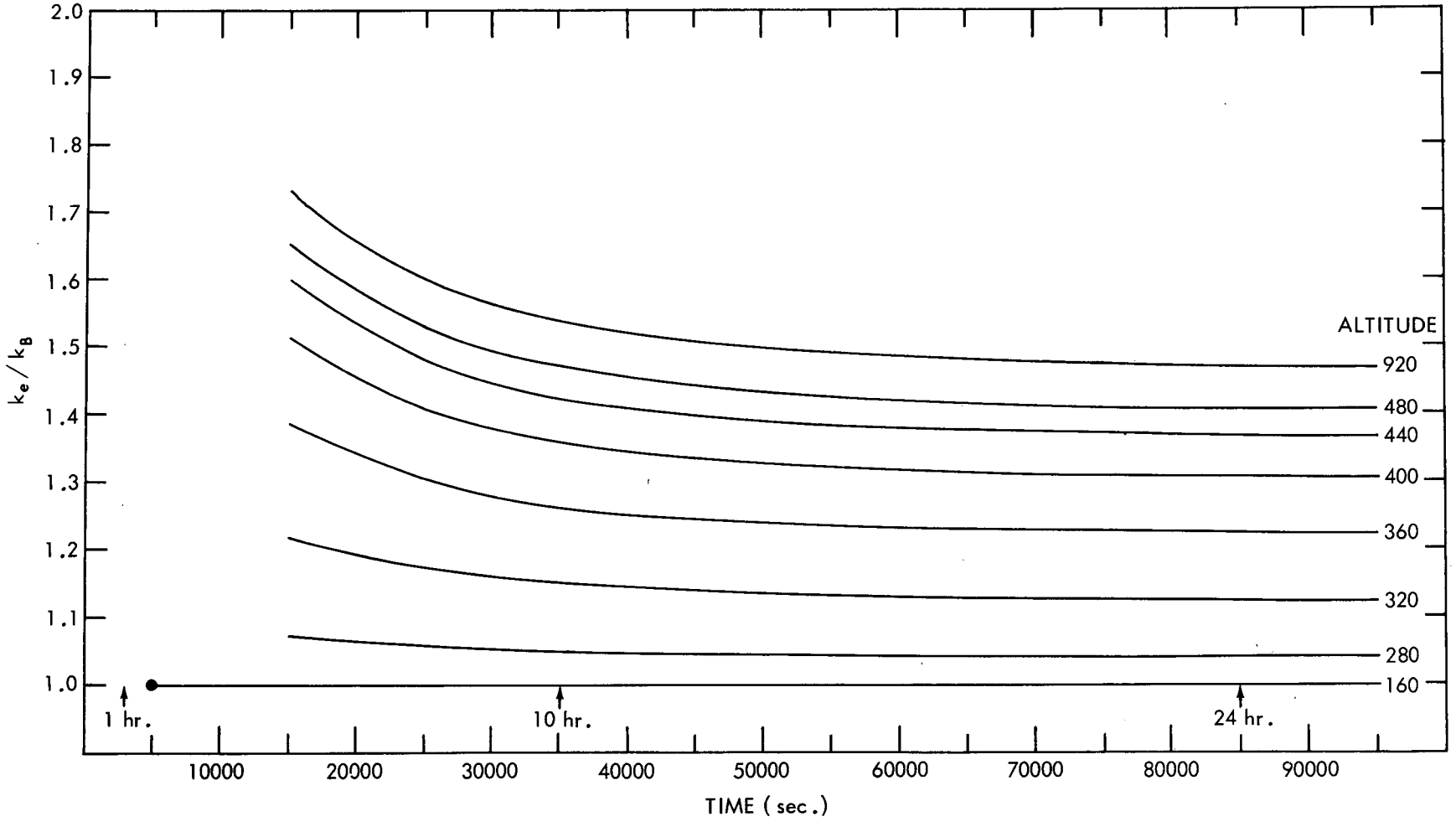

Figure 3-17. Ratio of the effective to the energetically equivalent reaction constant, k_e/k_B, versus time for several altitudes

$$k_e = \sum_{i=0} k(i) \frac{n_i}{n}$$
$$= \sum_{i=0} k(i) \frac{(n_i' + \epsilon_i)}{n} \qquad (3\text{-}1)$$

where k_e is the effective rate constant and k(i) is the rate constant for level i, taken from reference (13) and listed in Table 3. The reaction rate for the Boltzmann part of the solution, k_B, was calculated from equation (3-1) with the ϵ_i terms set to zero. The computer program for these calculations, REACTRAT, is listed in Appendix III. A comparison of k_e and k_B is a measure of the importance of the deviation from a Boltzmann distribution to the F_2 region ionospheric ionization loss.

Figure 3-17 shows the ratio k_e/k_B versus time for several altitudes of interest. It is apparent in the figure, that for altitudes above 320 km the ratio is significantly larger than 1 throughout the time interval of the solutions, and particularly during the first 10 hours, the approximate duration of SAR-arcs.

Figure 3-18 shows the ratio k_e/k_B versus altitude for five time steps. It is seen in the figure that for a given time step the ratio is relatively constant with altitude for altitudes above 500 km. There is a large variation of the ratio with altitude between 280 km and 500 km, the region of the atmosphere where diffusion becomes the dominant process. This figure shows that the deviations from a Boltzmann solution are noticeable for altitudes as low as 300 km.

Figures 3-19 and 3-20 show the effective rate constant, calculated from equation 3-1 using the ψ and ϕ_i equation solutions, versus time and altitude, respectively. These figures show that the rate constant can be factors of 2 to 8 times larger than

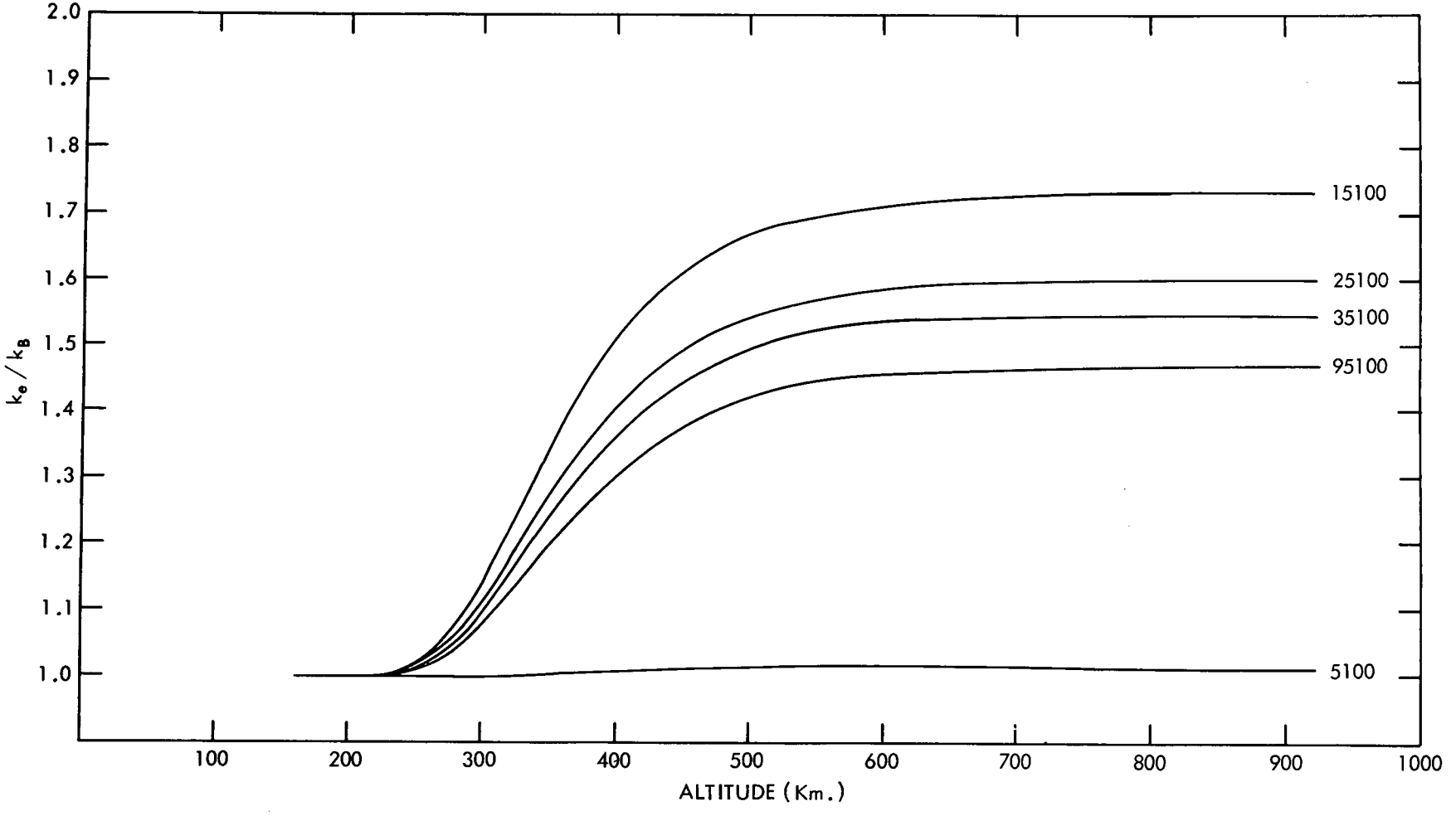

Figure 3-18. Ratio of the effective to the energetically equivalent reaction constant, k_e/k_B, versus altitude for five time steps

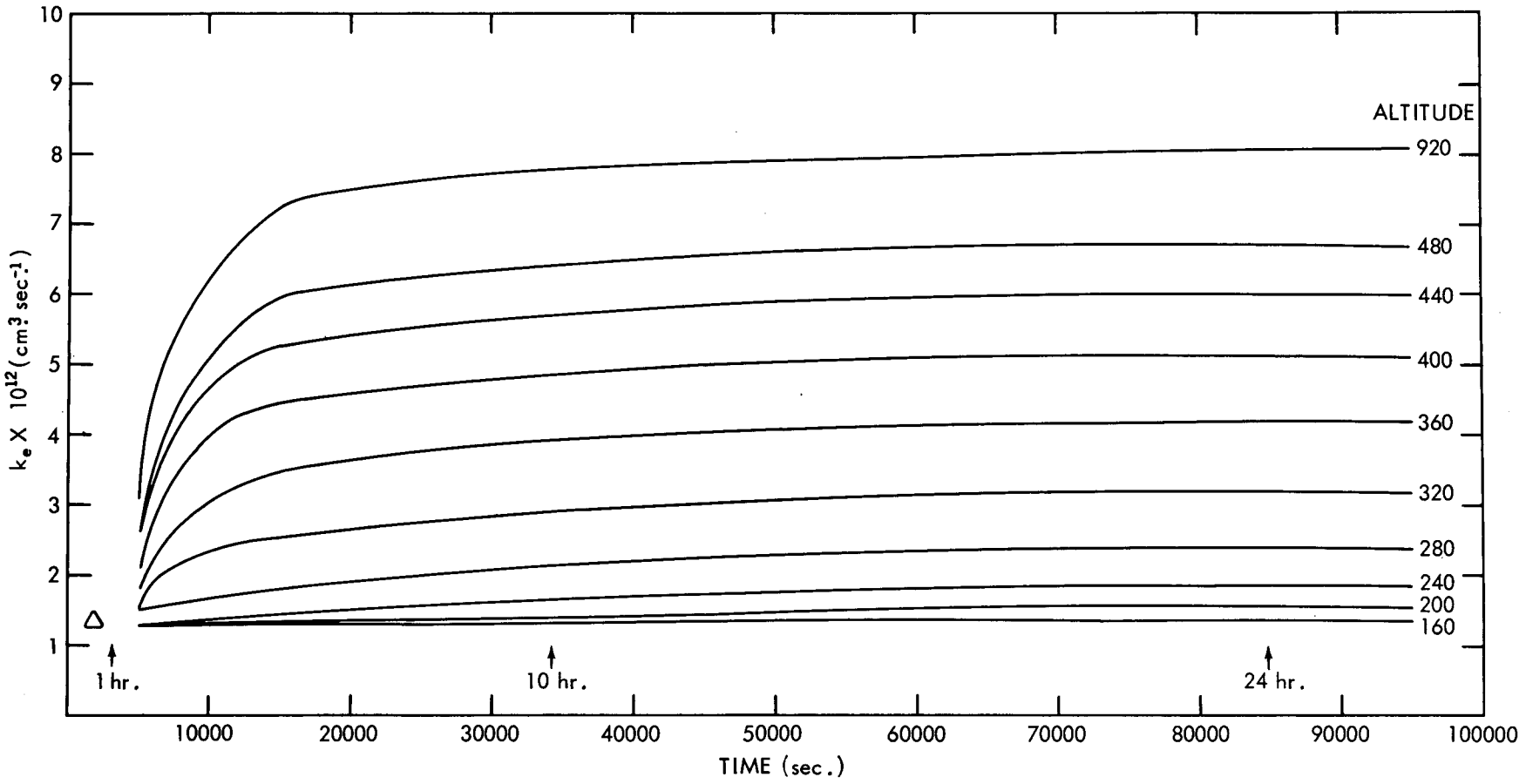

Figure 3-19. Effective reaction rate constant versus time for several altitudes

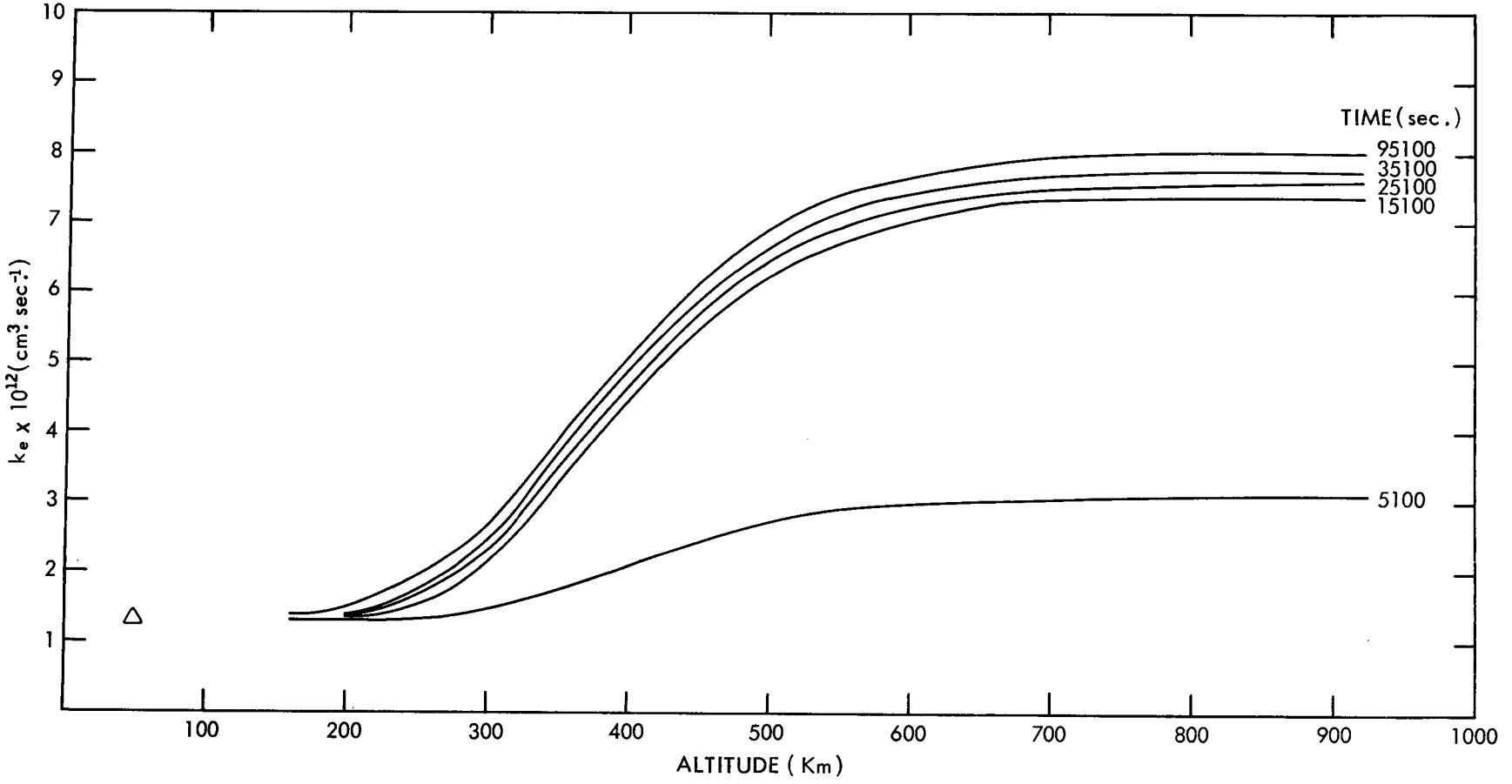

Figure 3-20. Effective reaction rate constant versus altitude for five time steps

the value for vibrational temperatures near 300°K (shown as a triangle in the two figures).

The k_e values, shown in Figures 3-19 and 3-20, have been used to calculate the loss rate for the ionospheric electrons and the ionospheric "loss time constant" in the following way. Assuming reaction (1-2) is infinitely fast, then the electron loss rate will be the same as the O^+ ion loss rate. Further assuming the electron density and the O^+ ion density are the same, we have

$$\frac{d n_e}{d t} = - k_e \, n \, n_e \tag{3-2}$$

where ne is the electron density. The loss rate for the electrons is defined from (3-2) to be

$$\frac{1}{\tau} = k_e \, n \tag{3-3}$$

where τ is the ionospheric loss time constant.

Figure 3-21 and 3-22 show the loss time constant calculated from (3-3) versus altitude and time respectively. In Figure 3-21 the loss rate for four time steps and the "normal" (vibrational temperature of 300°K) ionospheric time constant are shown. Noticeable decreases in the ionospheric loss time constant from the "normal" value is observed at altitudes as low as 280 km.

Figure 3-22 shows the loss time constant versus time for several altitudes where the time constant is one day or less. It is seen from the figure that in the first 10 hours, the time constant at 360 km. altitude, where the "normal" value is approximately 90 minutes, decreases to a value of 30 minutes. This figure shows

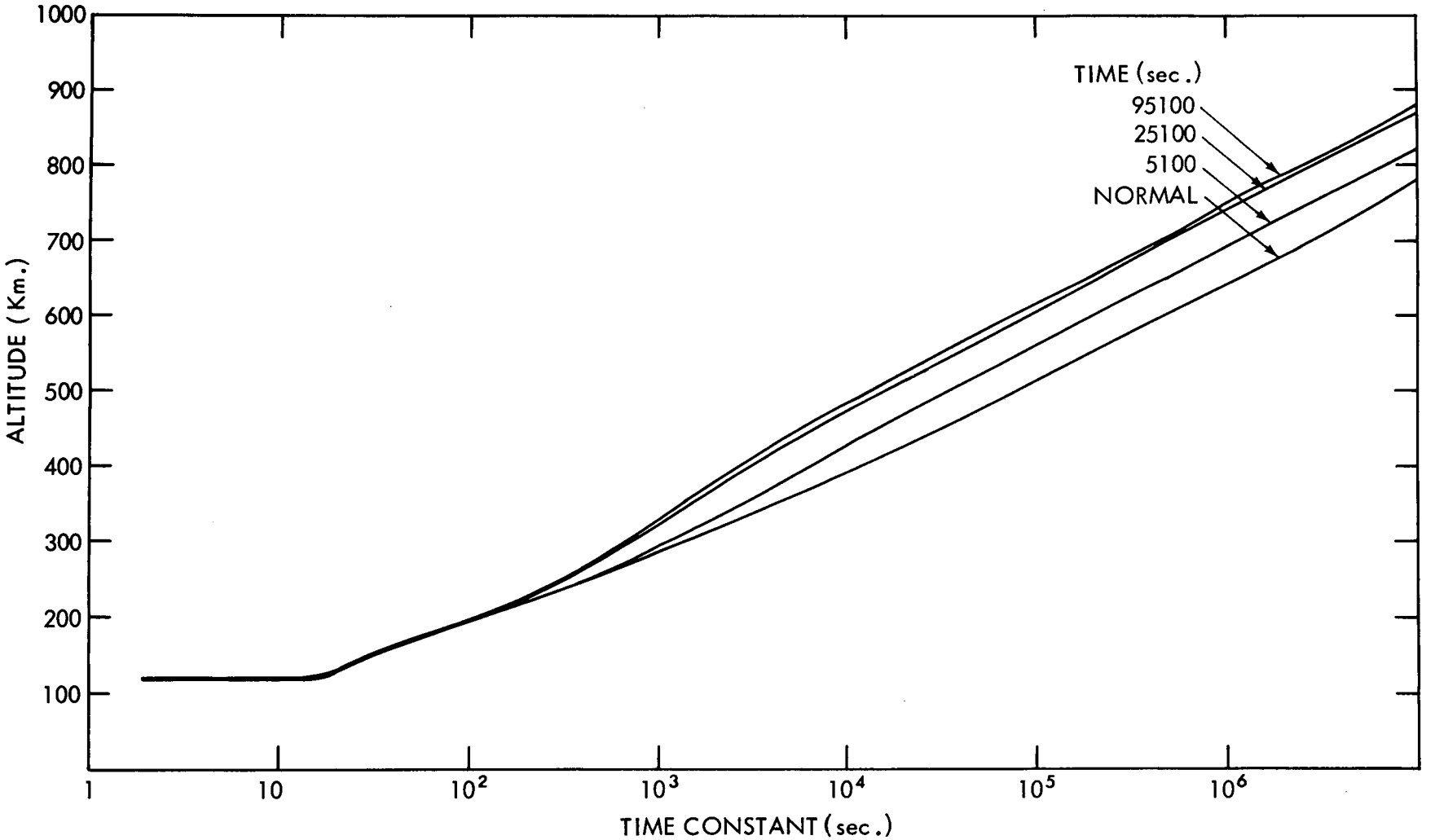

Figure 3-21. Ionospheric loss time constant versus altitude for four time steps

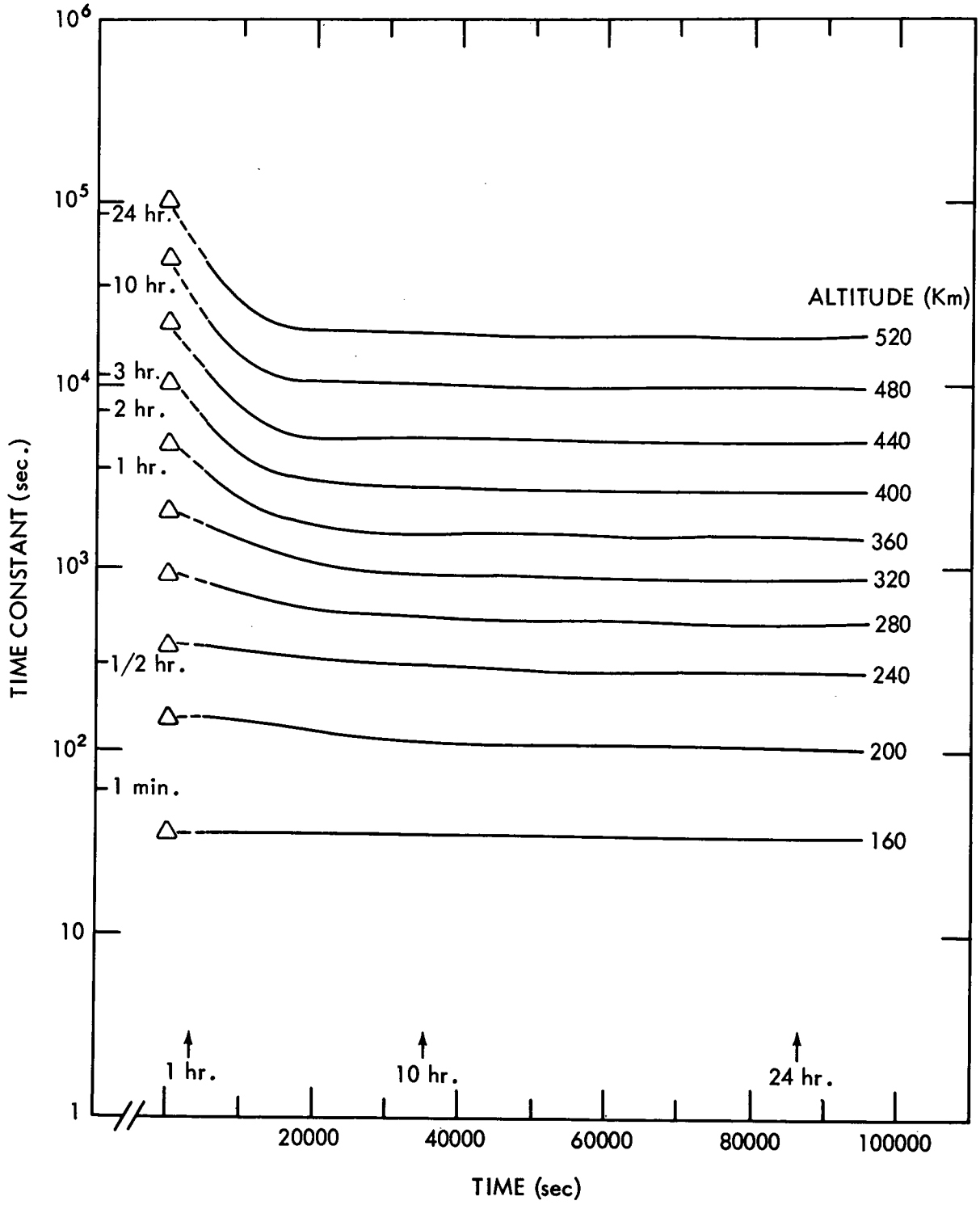

Figure 3-22. Ionospheric loss time constant versus time for altitudes where the time constant is 24 hours or less

that the ionospheric loss time constant is decreased by factors larger than three in altitude regions between 360 km and 440 km where the ionospheric loss time constant is measured in hours.

3.4 The effects of: neglect of ϵ_j /n; boundary conditions; and atomic oxygen loss process.

To determine the effect of the approximation of neglecting the ϵ_j /n term in the right hand side of the ψ equation, (A2-30), the solutions of the ϕ_i equations were used to calculate the ϵ_j /n terms. Equation (A2-30) was then solved using those ϵ_j /n terms. The second approximation to ψ was then used to recalculate the ϕ_i 's.

The second approximation to ψ yielded a vibrational temperature which was different from that obtained from the first approximation by 67°K, or less, at higher altitudes. At lower altitudes the difference was only a few degrees. The $\sum_{i=0}$ i ϵ_i terms from the new solutions were also reduced by as much as a factor of 3. Thus, as expected on the basis of the $\sum_{i=0}$ i ϵ_i results from the first solution, the second approximation to ψ produces only a few percent correction to the results of the first approximation. The ϵ_i 's calculated from the second approximation differed from those of the first approximation by 30%, or less, with most of the difference occurring at altitudes below 360 km. The $\sum_{i=0} \epsilon_i$ term changed by a few tens of percent only. It is concluded, that the second approximation produces a negligible correction to the ψ equation. Because most of the influence of the ϵ_i 's is at altitudes above 300 km. (see section 3.3), the second approximation to the ϵ_i 's is different from the first by only several percent in its impact on the ionospheric electron loss rates, and is therefore also negligible.

The ψ and ϕ_i equations were resolved using set 1 boundary conditions. It was found that the vibrational temperature calculated from the ψ equation solution differed from that obtained using set 2 boundary conditions by only a few degrees. The ϵ_i results differed by less than 3%. These results indicate that the solutions are not sensitive to the details of the loss mechanisms at the lower boundary.

An interesting result was obtained by comparing the behavior of the solutions with and without inclusion of the atomic oxygen production and loss processes for vibrational excitation, for set 1 boundary conditions (that is T_v (120, t) = T_v (z, 0) = 0°K). The solution including the oxygen process yielded vibrational temperatures that were larger at all altitudes than those obtained from solutions not including the atomic oxygen processes. The largest differences between the two solutions initially occurred at altitudes below 320 km and was greater than 150°K. This location for the differences is expected because this is the altitude region where the oxygen effects are relatively the most important. This result can be explained by the fact that the boundary condition of 0°K vibrational temperature causes the initial vibrational temperatures to be less than the gas temperature, thus the atomic oxygen is a source of vibrational excitation through translational-vibrational energy exchange. Eventually the electronic source of vibrational energy dominates the solution. In the "steady state" the vibrational temperature corresponding to the solution with no atomic oxygen processes has a vibrational temperature only 8°K greater at 160 km altitude and 6°K greater at 920 km altitude than that corresponding to the solution containing the atomic oxygen processes.

A comparison of the ϕ_i equation solutions for these two cases is complex. At altitudes below 280 km, the ϵ_i initially changed by factors as large as 30 and 40

with the largest values of ϵ_i corresponding to the solutions containing the oxygen processes. Above 320 km altitude the two solutions for the ϵ_i 's differ by approximately 25% or less. The ϵ_i 's of the upper two energy levels show the smallest differences between the two solutions. The two sets of solutions for the ϵ_i 's approach the same values in the steady state. The influence of the differences in the two sets of solutions on the ionospheric loss rates is small because the large differences occur below 320 km. altitude where the deviations from the Boltzmann part of the solutions play a small part in the determination of the reaction rate constant.

CHAPTER IV. SUMMARY AND CONCLUSIONS

The objective of this work was to determine if the observed decrease in ionospheric electron density occurring in SAR-arcs could be explained by an increase in the reaction constant for the rate determining ion-atom interchange reaction (1-1). The increase in the reaction constant is due to vibrational excitation of molecular nitrogen by subexcitation, inelastic collisions between ambient, thermal, electrons and nitrogen molecules. The finding of this work is that the vibrational excitation of molecular nitrogen is indeed important to the ionosphere under SAR-arc conditions and can cause the loss time constant for the F_2 region to change to lower values by factors of 1.6 to 5 with an attendant decrease in the electron density.

Previous work, (20), (22) on the related problem of the diurnal variation of the molecular nitrogen vibrational temperature assumed the vibrational distribution to be Boltzmann and considered diffusion processes. Earlier work (23) in the vertical distribution of vibrationally excited molecular nitrogen in aurora ignored diffusion and solved the continuity equations for the excited energy levels of molecular nitrogen. This work solves the continuity equations for the first six energy levels of molecular nitrogen including the diffusion process. Thus, it combines into one solution, the previous approaches.

The continuity equations to be solved are six, coupled, mildly non-linear, partial differential equations containing the dominant source and loss terms for vibrational excitation of molecular nitrogen. The solutions were divided into an energetically equivalent part that is Boltzmann distributed and a part representing deviations from the Boltzmann solution. The resulting equations were solved

numerically, using finite difference equations, to provide the populations of the energy levels as functions of time and altitude.

It was found, under conditions where the ionospheric electron temperature reaches values near 5000°K at 500 km altitude, that the vibrational temperature of molecular nitrogen reached a steady state value near 2300°K. at that altitude. The deviations from the Boltzmann distribution depends strongly on altitude for altitudes below 400 km. This is the region of the atmosphere where the diffusion process becomes dominant with increasing altitude over the vibrational-vibrational energy exchange process. It was found that for the highest three energy levels, above 300 km. altitude, the deviations from a Boltzmann distribution increased the populations of these levels by factors of 2 to 10. These results were insensitive to plausible variations of the boundary conditions.

The deviations from a Boltzmann distribution caused the effective reaction rate for reaction (1-1) to be increased by as much as a factor of 1.7 over the value obtained from the energetically equivalent Boltzmann solution. This indicates the possible importance of these deviations in problems involving chemical reactions at altitudes as low as 500 km. The effective reaction rate, calculated using the total population densities, was as much as a factor of 8 greater than the reaction rate for a vibrational temperature of 300°K. Significant enhancements of the reaction rate were found to occur at altitudes as low as 300 km.

Because of these increased reaction rates, the times required to significantly decrease the electron density in the ionosphere were reduced from their normal value by factors of 1.6 to 5, depending on altitude. Over most of the altitude range

where the loss time is short compared to SAR-arc durations, the loss time was reduced by factors exceeding 1.8.

These results lead to the conclusions that the vibrational excitation of molecular nitrogen, under conditions corresponding to SAR-arcs, causes a large increase in the loss rate of ionospheric electrons in the F_2 region. The enhanced loss rate is of such magnitude, that it alone will account for the observed electron density depressions in SAR-arcs.

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TABLE 1

Cross Sections used from Reference (30) in Equation (A1-19)

Cross-Section	Comment
σ_{10}	Numerical data available
σ_{20}	Numerical data available
σ_{03}	Numerical data available
σ_{04}	Numerical data available
σ_{50}	All that is available
σ_{12}	All that is available
σ_{13}	All that is available
σ_{14}	All that is available
σ_{51}	All that is available
σ_{23}	All that is available
σ_{24}	All that is available
σ_{52}	All that is available
σ_{34}	All that is available
σ_{53}	All that is available
σ_{54}	All that is available

TABLE 2

Parameters for Reaction Rate Constants for Production and

Loss of Vibrational Excitation by Electron Collisions

I.D.	P1	P2	P3	P4	Max Error %
10	-1.837483E01	-2.218530E04	1.684328E07	-4.558864E09	-19@2500°
20	-1.887149E01	-1.851033E04	-1.317388E06	2.310335E09	-37@1500°
50	-2.004471E01	-1.797215E04	-6.671288E06	2.076589E09	-14@2000°
51	-2.025835E01	-1.628830E04	-2.509007E06	7.790528E08	- 5@1500°
12	-1.874858E01	-1.222789E04	1.102594E07	-2.993175E09	14@5000°
52	-1.974898E01	-1.314905E04	-2.739562E06	9.167196E08	- 9@1500°
03	-1.950456E01	-5.705000E03	-6.362043E06	1.917276E09	-13@1500°
13	-1.972427E01	-4.652598E03	-6.585213E06	1.931419E09	-12@1500°
23	-1.939743E01	-8.030383E03	5.607227E06	-1.257535E09	-16@2000°
53	-1.980759E01	-8.800227E03	-2.526216E06	9.740170E08	-12@1500°
04	-1.964117E01	-3.913067E03	-5.735326E06	1.842685E09	-13@1500°
14	-2.019481E01	-3.588698E03	-4.862049E06	1.688892E09	- 9@1500°
24	-1.999716E01	-4.421176E03	-3.194914E06	1.243446E09	-10@1500°
35	-1.943835E01	-4.869426E03	2.078704E06	-1.935087E08	-15@1500°
54	-1.983298E01	-4.700520E03	-4.217622E05	4.723745E08	-14@1500°

TABLE 3

Reaction Rates for Vibrational Levels

Level	k_v [cm.^{3}sec.$^{-1}$]
0	1.3×10^{-12}
1	1.3×10^{-12}
2	5.0×10^{-11}
3	1.20×10^{-10}
4	2.6×10^{-10}
5	3.6×10^{-10}
6	4.4×10^{-10}
7	4.6×10^{-10}
8	4.6×10^{-10}
9	4.6×10^{-10}
10	4.6×10^{-10}
11	4.6×10^{-10}

APPENDIX I

ELECTRONIC PRODUCTION AND LOSS OF VIBRATIONAL EXCITATION

Production and loss rates for the first six vibrational levels of molecular nitrogen were calculated using theoretically calculated (28), (29), (30) cross-sections for inelastic, sub-excitation, electron scattering for these levels. The cross-sections were averaged over the Maxwell-Boltzmann energy distribution representing the electron gas to produce the production and loss rates. This section contains an amplified outline of the content of the theoretical cross-section calculations in Chen's, (28), (29) papers as well as discussion of the calculation of reaction rates.

Chen (28), (29) applies the unified theory of Feshbach (37), for nuclear reactions involving the formation of a compound state, to inelastic scattering of electrons by molecules. Herafter Chen (28) will be called paper I and equations contained therein referenced as I X.XX. Chen (29) will be referenced as paper II and equations contained therein will be referenced as II X.XX.

A1.1 Paper I:

Paper I starts with the consideration of an N-electron system consisting of an incident electron and a diatomic target molecule with N-1 electrons. The system is separated into relative and center of mass coordinates and the center of mass part is removed from the Schrodinger equation. The relative coordinates for the electrons, $\vec{X}, \vec{r}_1, \vec{r}_2 \ldots, \vec{r}_{N-1}$, are referenced to the center of mass of the nuclei. X refers to the incident electron. $\vec{R}$ is the vector separation of the two heavy nuclei a and b with masses M_a and M_b respectively. The Schrodinger

equation is (in atomic units)

$$[K_0(\vec{X}) + V_0(\vec{X}, \vec{r}, \vec{R}) + H_{ab}(\vec{r}, \vec{R})]\ \Omega = E\Omega \tag{I2.1}$$

where

$$V_0(\vec{x}, \vec{r}, \vec{R}) = \sum_{i=1}^{N-1} \frac{1}{|\vec{X} - \vec{r}_i|} - \frac{Z_a}{X_a} - \frac{Z_b}{X_b} \tag{I-2.2}$$

and $\vec{r}$ is the collective notation of $\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N-1}$ for the molecular electrons; K_0 is the kinetic energy operator of the incident electron; V_0 is the Coulombic potential energy of the incident electron; H_{ab} is the Hamiltonian for the target molecule; Ω is the total wavefunction for the system having the total energy E; X_a and X_b are the position vectors of the incident electron with respect to the two nuclei having Z_a and Z_b as their charges.

It is assumed that the unperturbed molecule is described by the set of Schrodinger equations

$$H_{el}(\vec{r}, \vec{R})\ \Phi_n(\vec{r}, \vec{R}) = \epsilon_n(R)\ \Phi_n(\vec{r}, \vec{R}) \tag{I-2.3}$$

$$[-(2\mu)^{-1}\ \nabla_R^2 + \epsilon_n(R)]\ \chi_{n\gamma}(\vec{R}) = \epsilon_{n\gamma}\ \chi_{n\gamma}(\vec{R}) \tag{I-2.4}$$

where

$$H_{el}(\vec{r}, \vec{R}) = \frac{1 + M_a + M_b}{2\ (M_a + M_b)} \sum_{i=1}^{N-1} \nabla_i^2 + U_{el}(\vec{r}, \vec{R}) \tag{I-2.5}$$

and

$$\mu = \frac{M_a M_b}{M_a + M_b};\quad \nabla_i^2$$

is the Laplacian operator on coordinate i and U_{el} is the potential energy of the molecular electrons.

$$H_{ab}(\vec{r},\ \vec{R}) = -\ (2\mu)^{-1}\ \nabla_R^2 + H_{el}\ (\vec{r},\ \vec{R}) \tag{I-2.6}$$

The cross terms for electrons and electron-nuclei contained in the Born-Oppenheimer separation are neglected because they do not enter, in the zeroth order approximation, in the expression for the excitation of nuclear motion, (34), pages 925-928. The electronic wavefunctions, Φ_n , and nuclear wavefunctions $\chi_{n\gamma}$ having eigenvalues ϵ_n (R) and $\epsilon_{n\gamma}$, respectively, form a complete, orthogonal set in their corresponding spaces.

The total wavefunction is expanded in terms of Φ_n and $\chi_{n\gamma}$ to give

$$\Omega(\vec{X},\ \vec{r},\ \vec{R}) = \sum_{n,\gamma} \Phi_n(\vec{r},\ \vec{R})\ \chi_{n\gamma}(\vec{R})\ \psi_{n\gamma}(\vec{X}) \tag{I-2.7}$$

where exchange effects are neglected. The expansion coefficients $\psi_{n\gamma}$ $(\vec{x})$ are assumed not to depend on the inter-nuclear separation as a parameter. It is assumed that the inter-nuclear separation is fixed at its equilibrium value $R_e^{(0)}$ for $\psi_{n\gamma}$ $(\vec{X})$. The effect of this assumption is estimated to be of order μ^{-1}.

Substituting equation (I-2.7) into the Schrodinger equation (I-2.1), multiplying on the left by $\Phi_{n'}^*$, $\chi_{n'\gamma'}^*$, integrating over $\vec{r}$ and $\vec{R}$ and using (I-2.3) through (I-2.6) we have the coupled sets of equations

$$[K_0(\vec{X}) + \epsilon_{n\gamma} - E]\ \psi_{n\gamma}(\vec{X}) = -\sum_{n',\gamma'} V_{nn'}^{\gamma\gamma'}(\vec{X})\ \psi_{n'\gamma'}(\vec{X}) \tag{I-2.8}$$

with

$$V_{nn'}^{\gamma\gamma'}(\vec{x}) = \langle \chi_{n\gamma} | V_{nn'}(\vec{X},\ \vec{R}) - (2\mu)^{-1}\ C_{nn'}(R,\ \nabla_R) | \chi_{n'\gamma'} \rangle \tag{I-2.9}$$

$$V_{nn'}(\vec{X},\ \vec{R}) = \langle \Phi_n | V_0(\vec{X},\ \vec{R},\ \vec{r}) | \Phi_{n'} \rangle \tag{I-2.10}$$

$$C_{nn'} = 2 \langle \Phi_n | \nabla_R | \Phi_{n'} \rangle \cdot \nabla_R + \langle \Phi_n | \nabla_R^2 | \Phi_{n'} \rangle \qquad \text{(I-2.11)}$$

Because we are interested in subexcitation electron impact, the $\psi_{0\gamma}$'s are of particular interest. Thus writing (I-2.8) as

$$[K_0(\vec{X}) + \epsilon_{0\gamma} - E]\, \psi_{0\gamma}(\vec{X}) = - \sum_{\gamma'} V_{00}^{\gamma\gamma'}\, \psi_{0\gamma'}(\vec{X}) - \sum_{\substack{n',\gamma' \\ n' \neq 0}} \psi_{n'\sigma}(\vec{X}) \qquad \text{(A1-1)}$$

and

$$[K_0(\vec{X}) + \epsilon_{n\gamma} - E]\, \psi_{n\gamma}(\vec{X}) = - \sum_{\gamma'} V_{n0}^{\gamma\gamma'}\, \psi_{0\gamma'}(\vec{X}) - \sum_{\substack{n',\gamma' \\ n' \neq 0}} V_{nn'}^{\gamma\gamma'}\, \psi_{n'\gamma'}(\vec{X}) \qquad \text{(A1-2)}$$

for $n \neq 0$.

Rewriting (1) and (2) we have

$$[K_0(\vec{X}) + \epsilon_{0\gamma}]\, \psi_{0\gamma}(\vec{X}) + \sum_{\gamma'} V_{00}^{\gamma\gamma'}\, \psi_{0\gamma'}(\vec{X}) - E\psi_{0\gamma}(\vec{X}) = - \sum_{\substack{n'\gamma' \\ n' \neq 0}} V_{0n'}^{\gamma\gamma'}\, \psi_{n'\gamma'}(\vec{X}) \qquad \text{(A1-3)}$$

$$[K_0(\vec{X}) + \epsilon_{n\gamma}]\, \psi_{n\gamma}(\vec{X}) + \sum_{\substack{n',\gamma' \\ n' \neq 0}} V_{nn'}^{\gamma\gamma'}\, \psi_{n'\gamma'}(\vec{X}) - E\psi_{n\gamma}(\vec{X}) = - \sum_{\gamma'} V_{n0}^{\gamma\gamma'}\, \psi_{0\gamma'}(\vec{X}) \qquad \text{(A1-4)}$$

Defining

$$T_n = \begin{bmatrix} K_0 + \epsilon_{n0} & & \\ & K_0 + \epsilon_{n1} & 0 \\ & & K_0 + \epsilon_{n2} \\ 0 & & \end{bmatrix} \qquad \text{(I-2.14)}$$

$$\psi_n = \begin{bmatrix} \psi_{n0} \\ \psi_{n1} \\ \psi_{n2} \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \qquad \text{(I-2.12)}$$

$$\Psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \qquad \text{(I-2.15)}$$

$$U_{nn'} = \begin{bmatrix} V_{nn'}^{00}, & V_{nn'}^{01}, & V_{nn'}^{02}, & \cdot & \cdot \\ V_{nn'}^{10}, & V_{nn'}^{11}, & V_{nn'}^{12}, & \cdot & \cdot \\ V_{nn'}^{20}, & V_{nn'}^{21}, & V_{nn'}^{22}, & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \qquad \text{(I-2.13)}$$

$$U_0 = (U_{01}, U_{02}, U_{03}, \cdots) \qquad \text{(I-2.16)}$$

$$U_0' = \begin{bmatrix} U_{10} \\ U_{20} \\ U_{30} \\ \cdot \\ \cdot \end{bmatrix} \qquad \text{(I-2.17)}$$

(3) and (4) become

$$T_0 \psi_0 + U_{00} \psi_0 - E\psi_0 = - \sum_{\substack{n' \\ n' \neq 0}} U_{0n'} \psi'_n = - U_0 \psi \qquad \text{(I-2.19)}$$

and

$$T_n \psi_n + \sum_{\substack{n' \\ n' \neq 0}} U_{nn'} \psi_{n'} - E\psi_n = - U_{n0} \psi_0$$

or

$$(H - E) \Psi = - U'_0 \psi_0 \qquad \text{(I-2.20)}$$

where

$$H = \begin{bmatrix} T_1 + U_{11} & U_{12} & U_{13} & \cdot & \cdot \\ U_{21} & T_2 + U_{22} & U_{23} & \cdot & \cdot \\ U_{31} & U_{32} & T_3 + U_{33} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \qquad \text{(I-2.18)}$$

and

$$E_{nn'} = E \delta_{nn'}$$

Following Fishbach's formalism, (37), the formal solution of (I-2.20) is

$$\Psi = (E - H + i\eta)^{-1} U'_0 \psi_0 \qquad \text{(I-2.21)}$$

where $\eta = \eta \delta_{ij}$ and $\eta \to 0^+$ to ensure outgoing waves in the exit channels, (I-2.21) gives ψ in terms of ψ_0. Using (I-2.21) in (I-2.19), we obtain

$$(T_0 + \Lambda - E) \psi_0 = 0 \qquad \text{(I-2.22)}$$

where

$$\Lambda = U_{00} + U_0 (E - H + i\eta)^{-1} U_0' \tag{I-2.23}$$

and is the effective scattering potential for subexcitation scattering of electrons by molecules.

The formal solution (I-2.21) contains the Green's function operator $\lim_{n\to 0^+} (E_1 - H + i\eta)^{-1}$ which implies the need for a set of eigenfunctions of the effective Hamiltonian H. Thus we write

$$H\Psi_m = W_m \Psi_m \tag{I-3.2}$$

where a set of eigenfunctions $\{\Psi_m\}$ approximates the set of compound negative ion eigenfunctions with energy spectrum $\{W_m\}$.

The physical significance of these states is illustrated in the weak coupling limit where H is diagonal. In this case (I-3.2) gives the equations

$$(T_n + U_{nn})\, \psi_n^{(m)} = W_n^{(m)}\, \psi_n^{(m)} \qquad n \neq 0 \tag{I-3.3}$$

which is expanded further to become

$$[K_0 + V_{nn}^{\gamma\gamma} + \epsilon_{n0} - W_{n\gamma}^{(m)}]\, \psi_{n\gamma}^{(m)} = - \sum_{\gamma' \neq \gamma} V_{nn}^{\gamma\gamma'} \psi_{n\gamma'}^{(m)} \tag{I-3.4}$$

The compound negative ion states $\psi_n^{(m)}$ describe, in this instance, a set of states of the incident electron in resonance with the field of the excited target molecule.

Expanding the Green's function operator contained in (I-2.21) in terms of the eigenfunctions Ψ_m we have

$$G^{(+)}(E) = \sum_m \frac{|\Psi_m\rangle\langle\Psi_m|}{E - W_m} + \int d\rho \int dW \frac{|\Psi(\rho, W)\rangle\langle\Psi(\rho, W)|}{E - W + i\eta} \qquad \text{(I-4.1)}$$

where the sum over m is for the discrete states and the integral over ρ contains the continuous eigenspectrum for energy E. Expression (I-4.1) implies a resonance part of the operator and a non-resonance part. Therefore we write

$$G^{(+)}(E) = Q(E) + G_0^{(+)}(E) \qquad \text{(I-4.2)}$$

with

$$Q(E) = \sum_m \frac{|\Psi_m\rangle\langle\Psi_m|}{E - W_m} \qquad \text{(I-4.3)}$$

Q(E) is the resonance part of the operator and the prime means that only those negative ion states having energies comparable to that of the system are included in the summation. The effective potential (I-2.23) is now written, using (I-4.2) in (I-2.23) as

$$\Lambda = u' + u \qquad \text{(I-4.4)}$$

where

$$u' = U_0 Q(E) U_0' \qquad \text{(I-4.5)}$$

$$u = U_{00} + U_0 G_0^{(+)}(E) U_0' \qquad \text{(I-4.6)}$$

Let $\pi_0^{(-)}$ be the solution for an outgoing wave of the equation

$$(T_0 - E)\, \pi_0^{(-)} = 0$$

Using (I-4.4) in (I.22) we have

$$(T_0 + U - E)\,\psi_0 = -\,u'\,\psi_0 \tag{A1-5}$$

where the resonance part of the effective scattering potential is treated as the scattering potential.

From scattering theory, (38), Chapter 12, the solution for the outgoing wave is

$$\psi_0 = \psi_0^{(+)} + (E - T_0 - u + i\eta)^{-1}\,u'\,\psi_0 \tag{I-4.12}$$

where

$$(T_0 + u - E)\,\psi_0^{(+)} = 0 \tag{I-4.10}$$

and $\psi_0^{(+)}$ is an incoming wave and contains the effects of the direct scattering potential u.

The transition matrix describing transitions from the incident channel γ' to channel γ for n = 0 is

$$\mathfrak{I}_0(\gamma, \gamma') = \langle \pi_0^{(-)}(\gamma)\ |u + u'|\ \psi_0(\gamma') \rangle \tag{I-4.13}$$

Consider the outgoing wave solutions to

$$(T_0 + u - E)\,\psi_0^{(-)} = 0 \tag{A1-6}$$

which may be written as

$$\psi_0^{(-)} = \pi_0^{(-)} + (E - T_0 - i\eta)^{-1}\,u\psi_0^{(-)} \tag{I-4.14}$$

Multiplying by $(E - T_0 - i\eta)$ and adding and subtracting $u\pi_0^{(-)}$ to the right hand side we have

$$(E - T_0 - i\eta)\,\psi_0^{(-)} = (E - T_0 - i\eta)\,\pi_0^{(-)} + u\psi_0^{(-)} + u\pi_0^{(-)} - u\pi_0^{(-)} \tag{A1-7}$$

$$\therefore\ \psi_0^{(-)} = \pi_0^{(-)} + (E - T_0 - u - i\eta)^{-1}\, u\, \pi_0^{(-)} \tag{I-4.15}$$

$$\therefore\ \pi_0^{(-)} = \psi_0^{(-)} - (E - T_0 - u - i\eta)\, u\pi_0^{(-)} \tag{A1-8}$$

Substituting (A-1-8) in (I-4.13) we have

$$\begin{aligned}\mathfrak{I}_0(\gamma, \gamma') &= \langle \pi_0^{(-)} |u|\ \psi_0\rangle - \langle (E - T_0 - u - i\eta)^{-1}\, u\pi_0^{(-)} |u'|\ \psi_0\rangle \\ &\quad + \langle \psi_0^{(-)} |u'|\ \psi_0\rangle \end{aligned} \tag{I-4.16}$$

$$\begin{aligned}&= \langle \pi_0^{(-)} |u|\ \psi_0 - (E - T_0 - u + i\eta)^{-1}\, u'\ \psi_0\rangle \\ &\quad + \langle \psi_0^{(-)} |u'|\ \psi_0\rangle \end{aligned} \tag{A1-9}$$

$$= \langle \pi_0^{(-)} |u|\ \psi_0^{(+)}\rangle + \langle \psi_0^{(-)} |u'|\ \psi_0\rangle \tag{I-4.17}$$

using (I-4.12). Consider $\langle \psi_0^{(-)} |u'|\ \psi_0\rangle$ and repeatedly substitute (I-4.12) for ψ_0 to obtain

$$\begin{aligned}\langle \psi_0^{(-)} |u'|\ \psi_0\rangle &= \langle \psi_0^{(-)} |u'|\ \psi_0^{(+)}\rangle + \langle \psi_0^{(-)} |u'(E - T_0 - u + i\eta)^{-1}\, u'\ |\psi_0\rangle \\ &= \langle \psi_0^{(-)} |u'|\ \psi_0^{(+)}\rangle + \langle \psi_0^{(-)} |u'\,(E - T_0 - u + i\eta)^{-1}\, u'\ |\psi_0^{(+)}\rangle \\ &\quad + \langle \psi_0^{(-)} |u'(E - T_0 - u + i\eta)^{-1}\, u(E - T_0 - u + i\eta)^{-1}\, u'\ |\psi_0^{+}\rangle \\ &\quad + \cdots \\ &= \langle \psi_0^{(-)} |u' + u'\,(E - T_0 - u + i\eta)^{-1}\, u' + u'\,(E - T_0 - u + i\eta)^{-1}\, u' \\ &\quad \cdot (E - T_0 - u + i\eta)^{-1}\, u' + \cdots |\psi_0^{(+)}\rangle \end{aligned} \tag{A1-10}$$

For an isolated resonance, the summation over m in (I-4.3) reduces to one term and (I-4.5) becomes

$$u' = \frac{U_0 \, |\Psi_m\rangle\langle\Psi_m| \, U_0'}{E - W_m} \tag{A1-11}$$

Thus (11) becomes

$$\langle\psi_0^{(-)}|u'|\psi_0\rangle = \frac{\langle\psi_0^{(-)}|U_0|\Psi_m\rangle\langle\Psi_m|U_0'|\psi_0^{(+)}\rangle}{E - W_m} \left\{1 + \frac{\langle\Psi_m|U_0'(E - T_0 - u + i\eta)^{-1} U_0 \Psi_m\rangle}{E - W_m} + \cdots\right\}$$

Let

$$R_m = \langle\Psi_m|U_0'(E - T_0 - u + i\eta)^{-1} U_0|\Psi_m\rangle \tag{I-4.23}$$

Therefore

$$\langle\psi_0^{(-)}|u'|\psi_0\rangle = \frac{\langle\psi_0^{(-)}|U_0|\Psi_m\rangle\langle\Psi_m|U_0'|\psi_0^{(+)}\rangle}{E - W_m} \left\{1 + \frac{R_m}{E - W_m} + \frac{R_m^2}{E - W_m} + \cdots\right\}$$

$$= \frac{\langle\psi_0^{(-)}|U_0|\Psi_m\rangle\langle\Psi_m|U_0'|\psi_0^{(+)}\rangle}{E - W_m - R_m} \tag{I-4.24}$$

A1.2 Paper II.

In his application to molecular nitrogen, (29), Chen makes the following assumptions:

(1) an isolated resonance occurs.

(2) the direct transition amplitude is negligible.

(3) a single excited electronic state, n, of the target molecule is responsible for the resonance.

(4) the nuclear states of the target molecule are not strongly coupled and the Born-Oppenheimer coupling matrix elements are negligible.

(5) the total contribution to the transition amplitudes due to resonance effects of the set of compound negative-ion states may be accounted for as a linear sum of the individual contribution of each compound state.

From assumptions (1) and (2) equation (I-4.24) gives the transition matrix element. Thus

$$\mathfrak{I}_0(\gamma, \gamma') = \frac{\langle \psi_0^{(-)}(\gamma) \; |U_0| \; \Psi_m \rangle \langle \Psi_m \; |U_0'| \; \psi_0^{(+)}(\gamma') \rangle}{E - W_m - R_m} \qquad \text{(II-2.2)}$$

From assumption (3) only V_{on}, V_{no}, V_{nn} and V_{oo} in equation (I-2.10) are non-zero. Thus H in equation (I-2.18) becomes a single element matrix. Assumption (4) gives from equations (I-2.11) and (I-2.9) respectively

$$C_{nn'} = 0 \quad \text{and} \quad V_{nn}^{\gamma\gamma'} = 0 .$$

Thus U_{nn} in equation (I-2.13) is diagonal. Therefore we have

$$H\Psi_m = W_m \Psi_m$$

giving

$$H_n \psi_n^{(m)} = W_n^{(m)} \psi_n^{(m)}$$

or

$$(T_n + U_{nn}) \psi_n^{(m)} = W_n^{(m)} \psi_n^{(m)} \qquad \text{(A1-12)}$$

where

$$\psi_n^{(m)}(\lambda) = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \psi_{n\lambda}^{(m)} \\ 0 \\ \cdot \\ \cdot \end{bmatrix}$$

Expanding (A1-12) further and rearranging terms

$$[K_0 + V_{nn}^{\lambda\lambda}]\ \psi_{n\lambda}^{(m)} = (W_{n\lambda}^{(m)} - \epsilon_{n0})\ \psi_{n\lambda}^{(m)}$$

$$\equiv \{\epsilon_{n\lambda}^{(m)} - \epsilon_n(R_e^{(m)})\}\ \psi_{n\lambda}^{(m)} \qquad \text{(II-2.4)}$$

Now consider

$$(U_0\ |\psi_m\rangle)_\gamma = \left(\sum_r U_{0r}\ \psi_r^{(m)}\right)_\gamma$$

$$= (U_{0n}\ \psi_n^{(m)})_\gamma$$

$$= V_{0n}^{\gamma\lambda}\ \psi_{n\lambda}^{(m)} \qquad \text{(A1-13)}$$

Similarly

$$(U_0'^{\dagger}\ |\psi_m\ )_\gamma = V_{on}^{\gamma'\lambda\dagger}\ \psi_{n\lambda}^{(m)} \qquad \text{(A1-14)}$$

The $\gamma' \to \gamma$ transition due to the λ th vibrational level in the negative ion state is

$$\mathfrak{I}_0^\lambda(\gamma, \gamma') = \frac{\langle\psi_{0\gamma}^{(-)}\ |V_{0n}^{\gamma\lambda}|\ \psi_{n\lambda}^{(m)}\rangle\ \langle\psi_{n\lambda}^{(m)}|V_{n0}^{\lambda\gamma'}|\ \psi_{0\gamma'}^{(+)}\rangle}{E - W_{n\lambda}^{(m)} + R_{n\lambda}^{(m)}}$$

Using assumption (5), the total transition matrix element is

$$\mathfrak{I}_0(\gamma, \gamma') = \sum_\lambda \mathfrak{I}_0^\lambda(\gamma, \gamma')$$

$$= \sum_\lambda \frac{\langle \psi_{0\gamma}^{(-)} | V_{0n}^{\gamma\lambda} | \psi_{n\lambda}^{(m)} \rangle \langle \psi_{n\lambda}^{(m)} | V_{n0}^{\lambda\gamma'} | \psi_{0\gamma'}^{(+)} \rangle}{E - W_{n\lambda}^{(m)} + R_{n\lambda}^{(m)}} \qquad \text{(II-2.3)}$$

And

$$R_{n\lambda}^{(m)} = \langle \psi_{n\lambda}^{(m)} | \sum_\gamma V_{n0}^{\lambda\gamma} (E - H_0 + i\eta)^{-1} V_{0n}^{\gamma\lambda} | \psi_{n\lambda}^{(m)} \rangle \qquad \text{(II-2.5)}$$

Expanding

$$(E - H_0 + i\eta)^{-1} = \int dE_\gamma \frac{|\psi_{0\gamma}^{(+)}\rangle \langle \psi_{0\gamma}^{(-)}|}{E - E_\gamma + i\eta} \xi_\gamma$$

where ξ_γ is the density of states in the exit channel γ, and using

$$\frac{1}{E - E_\gamma + i\eta} = \frac{E - E_\gamma}{(E - E_\gamma)^2 + \eta^2} - \frac{i\eta}{(E - E_\gamma)^2 + \eta^2}$$

we have

$$R_{n\lambda}^{(m)} = \Delta_{n\lambda}^{(m)} - i\frac{1}{2}\Gamma_{n\lambda}^{(m)} \qquad \text{(II-2.5)}$$

where

$$\Delta_{n\lambda}^{(m)} = \langle \psi_{n\lambda}^{(m)} \left| \sum_\gamma P \int V_{n0}^{\lambda\gamma} \frac{E - E_\gamma}{(E - E_\gamma)^2 + \eta^2} \right| \psi_{0\gamma}^{(+)} \rangle \langle \psi_{0\gamma}^{(-)} | V_{0n}^{\gamma\lambda} \xi_\gamma \, dE_\gamma | \psi_{n\lambda}^{(m)} \rangle \qquad \text{(II-2.8)}$$

and

$$\Gamma^{(m)}_{n\lambda} = 2\ \mathrm{Im}\ (R^{(m)}_{n\lambda})$$

$$= 2\ \langle \psi^{(m)}_{n\lambda} \Big| \sum_{\gamma} \int V^{\lambda\gamma}_{n0}\ \frac{\eta\ |\psi^{(+)}_{0\gamma}\rangle \langle \psi^{(-)}_{0\gamma}|}{(E - E_\gamma)^2 + \eta^2}\ V^{\gamma\lambda}_{on}\ \xi_\gamma\ dE_\gamma \Big|\ \psi^{(m)}_{n\lambda}\rangle \qquad \text{(A1-15)}$$

$$= 2\ \langle \psi^{(m)}_{n\lambda} \Big| \sum_{\gamma} \int V^{\lambda\gamma}_{n0}\ |\psi^{(+)}_{0\gamma}\rangle \langle \psi^{(+)}_{0\gamma}\rangle\ \langle \psi^{(-)}_{0\gamma}|\pi\,\delta(E - E_\gamma)\ V^{\gamma\lambda}_{0n}\ \xi_\gamma\ dE_\gamma \Big|\ \psi^{(m)}_{n\lambda}\rangle \qquad \text{(A1-16)}$$

Using

$$\xi_\gamma = \frac{d\Omega_f}{(2\pi)^3}\ \frac{k_\gamma d\,(k^2_\gamma)}{dE_\gamma}$$

$$= \frac{d\Omega_f}{(2\pi)^3}\ \frac{1}{2}\ \frac{k_\gamma d(k^2_\gamma)}{dE_\gamma}$$

and

$$E_\gamma = \frac{1}{2} k^2_\gamma$$

then

$$\xi_\gamma = \frac{d\Omega_f}{(2\pi)^3}\ k_\gamma \qquad \text{(A1-17)}$$

Using (A1-17) to (A1-16) we have

$$\Gamma^{(m)}_{n\lambda} = \frac{1}{(2\pi)^2} \sum_{\gamma} \int |\langle\ \psi^{(-)}_{0\gamma} | V^{\gamma\lambda}_{0n} | \psi^{(m)}_{n\lambda}\rangle\ |^2\ k_\gamma\ d\Omega_f \qquad \text{(II-2.9)}$$

Using the definitions of $V^{\gamma\lambda}_{0n}$ and $V^{\lambda\gamma'}_{n0}$ from equation (I-2.10) and interchanging the order of integration in (II-2.3) we obtain

$$\mathfrak{I}_0(\gamma, \gamma') = \sum_{\lambda} \frac{\langle \chi_{0\gamma} | \alpha_{\gamma\lambda} |\ \chi_{n\lambda}\rangle \langle \chi_{n\lambda} | \alpha^*_{\lambda\gamma'} | \chi_{0\gamma'}\rangle}{E - E^{(m)}_{n\lambda} + i\,1/2\,\Gamma^{(m)}_{n\lambda}} \qquad \text{(II-2.11)}$$

and

$$\Gamma_{n\lambda}^{(m)} = \sum_{\gamma} \frac{k_\gamma}{(2\pi)^2} \int |\langle \chi_{0\gamma} | a_{\gamma\lambda} | \chi_{n\lambda} \rangle|^2 \, d\Omega_f \qquad \text{(II-2.12)}$$

where

$$a_{\gamma\lambda} = \langle \psi_{0\gamma}^{(-)} \, \Phi_0 | V_0 | \, \Phi_n \, \psi_{n\lambda}^{(m)} \rangle \qquad \text{(II-2.13a)}$$

$$a_{\lambda\gamma}^{*} = \langle \psi_{n\lambda}^{(m)} \, \Phi_n \, | V_0 | \, \Phi_0 \, \psi_{0\lambda'}^{(+)} \rangle \qquad \text{(II-2.13b)}$$

$$E_{n\lambda}^{(m)} = W_{n\lambda}^{(m)} + \Delta_{n\lambda}^{(m)} = \epsilon_{n\lambda}^{(m)} + \Delta_{n\lambda}^{(m)} + \epsilon_{n\lambda} - \epsilon_n(R_e^{(n)}) \qquad \text{(II-2.14)}$$

The differential partial cross section $d\sigma_{\gamma\gamma'}$, is expressed as a function of the incident angles of the impinging electron by

$$d\sigma_{\gamma\gamma'} = (4\pi^2)^{-1} \, |\mathfrak{I}_0(\gamma, \, \gamma')|^2 \, d\Omega_f$$

where

$$k_\gamma^2 = k_{\gamma'}^2 + 2(\epsilon_{0\gamma'} - \epsilon_{0\gamma})$$

with the initial and final wavenumbers of the electron given by $k_{\gamma'}$ and k_γ respectively.

Because the rotational motion of the molecule is relatively slow, the molecular orientation is considered fixed throughout the vibrational excitation or de-excitation. If the molecule remains in the ground rotational state then the partial cross-section can be obtained by averaging the transition matrix elements over the incident angles and integrating the resultant over the sphere of the final angles. The result is

$$\sigma_{\nu\nu'} = (16\pi^3)^{-1} \frac{k_\nu}{k_{\nu'}} \iint |\mathfrak{I}_0(\nu, \, \nu')|^2 \, d\Omega_0 \, d\Omega_f \qquad \text{(II-2.17)}$$

where the γ's have been replaced by ν's to reflect that the χ's now represent vibrational wave functions only.

The further assumption that the compound negative-ion state does not depend on the vibrational state is made. This assumption allows the cross-section to be written as

$$\sigma_{\nu\nu'} = \frac{\beta_\nu \beta_{\nu'}}{16\pi^3} \frac{k_\nu}{k_{\nu'}} \left| \sum_\lambda \frac{\langle \chi_{0\nu} | \chi_{n\lambda} \rangle \langle \chi_{n\lambda} | \chi_{0\nu'} \rangle}{E - E_{n\lambda}^{(m)} + i\frac{1}{2}\Gamma_{n\lambda}^{(m)}} \right|^2 \tag{II-2.18}$$

with

$$\Gamma_{n\lambda}^{(m)} = \sum_\nu \beta_\nu k_\nu (2\pi)^{-2} |\langle \chi_{0\nu} | \chi_{n\lambda} \rangle|^2 \tag{II-2.19}$$

$$\beta_\nu = \int |\alpha_{\nu 0}|^2 \, d\Omega_f \tag{II-2.20}$$

$$\beta'_\nu = \int |\alpha_{0\nu'}|^2 \, d\Omega_0 \tag{II-2.21}$$

$$E_{n\lambda}^{(m)} = \epsilon_{n0}^{(m)} + \Delta_{n0}^{(m)} + \epsilon_{n\lambda} - \epsilon_n (Re^{(n)}) \tag{II-2.22}$$

where the α's have been taken outside of the R integrals because they vary slowly and most of their contribution comes from a narrow range of internuclear separation $R = Re^{(0)}$.

Chen used Morse anharmonic wavefunctions for the χ's and approximated the resonance energy (II-2.22) by

$$E_{n\lambda}^{(m)} = \epsilon_{n0}^{(m)} + \Delta_{n0}^{(m)} + \left(\lambda + \frac{1}{2}\right) \omega_e^{(n)} - \left(\lambda + \frac{1}{2}\right)^2 \omega_e^{(n)} x_e^{(n)} \tag{II-3.3}$$

where $\omega_e^{(n)}/2$ is the zero point energy of the corresponding harmonic oscillator and the last term is an anharmonic correction. The β's are found from the set of linear equations (II-2.19). The cross sections are then determined from (II-2.18).

The excited field for resonance was identified as the $x^1 \Sigma_g^-$ of N_2. Once the excited state is identified the energy scale and averaged peak widths are shifted and altered by varying two parameters $\epsilon_{n0}^{(m)} + \Delta_{n0}^{(m)}$ and $\Gamma_{n0}^{(m)}$ until adjustment to the experimental data is achieved. The values giving the best fit are

$$\epsilon_{n0}^{(m)} + \Delta_{n0}^{(m)} = 1.89 \text{ ev}$$

$$\Gamma_{n0}^{(m)} = 0.152 \text{ e v}$$

These values are then used in the calculation of the cross-sections for excitation and de-excitation for other levels. (See reference (30) for the corrected figures for reference (29).)

A1.3 Calculation of reaction rates:

The reaction rate I_{ij}, is obtained from the cross section, σ_{ij}, by

$$I_{ij} = \iiint_{-\infty}^{\infty} v_e \, \sigma_{ij} (v_e) \, f (v_e) \, d^3 v_3 \qquad \text{(A1-18)}$$

where

v_e is the electron velocity

$f (v_e)$ is the distribution function for the electrons (assumed Maxwell-Boltzmann).

Equation (A1-18) when expressed in terms of electron energy, E in Ev, becomes

$$I_{ij} = (1.26574 \times 10^{-6})\,\pi\left(\frac{2}{\pi\, k\, Te}\right)^{3/2} \frac{1}{\sqrt{m_e}} \int_0^\infty E\sigma_{ij}(E)\, e^{-E/kTe}\, dE \quad \text{(A1-19)}$$

where m_e is the electron mass in grams.

Te is the electron temperature in °K

k is Boltzmann's constant.

Chen presents, in graphical form, the cross sections which allow calculation of (A1-19) for all transitions among the first five excited levels of N_2. Because we are concerned with moderate electron temperatures, the low energy regions of the cross sections are of particular interest. By using (A1-19) and detailed balancing arguments we may relate the cross sections for excitation and de-excitation in the following way

$$\sigma_{ji}(E - \epsilon_{ij}) = \frac{E}{E - \epsilon_{ij}}\, \sigma_{ij}(E) \quad \text{(A1-20)}$$

where ϵ_{ij} is the threshold for the j→ i transition. Thus, near threshold we should use de-excitation cross sections in (A1-19) because the low energy tails are more readily observed. The principal of detailed balance allows calculation of the excitation reaction rate from

$$I_{ji} = I_{ij}\, e^{-(Ej-Ei)/kT_e} \quad \text{(A1-21)}$$

The cross-section graphs in Chen's paper (30) were digitized and numerical integration of (A1-19) was performed for electron temperatures between 500°K and 10000°K. The identification of the cross sections used are given in Table (1). The calculated reaction rates are plotted in Figures A1-1 through A1-15 as points.

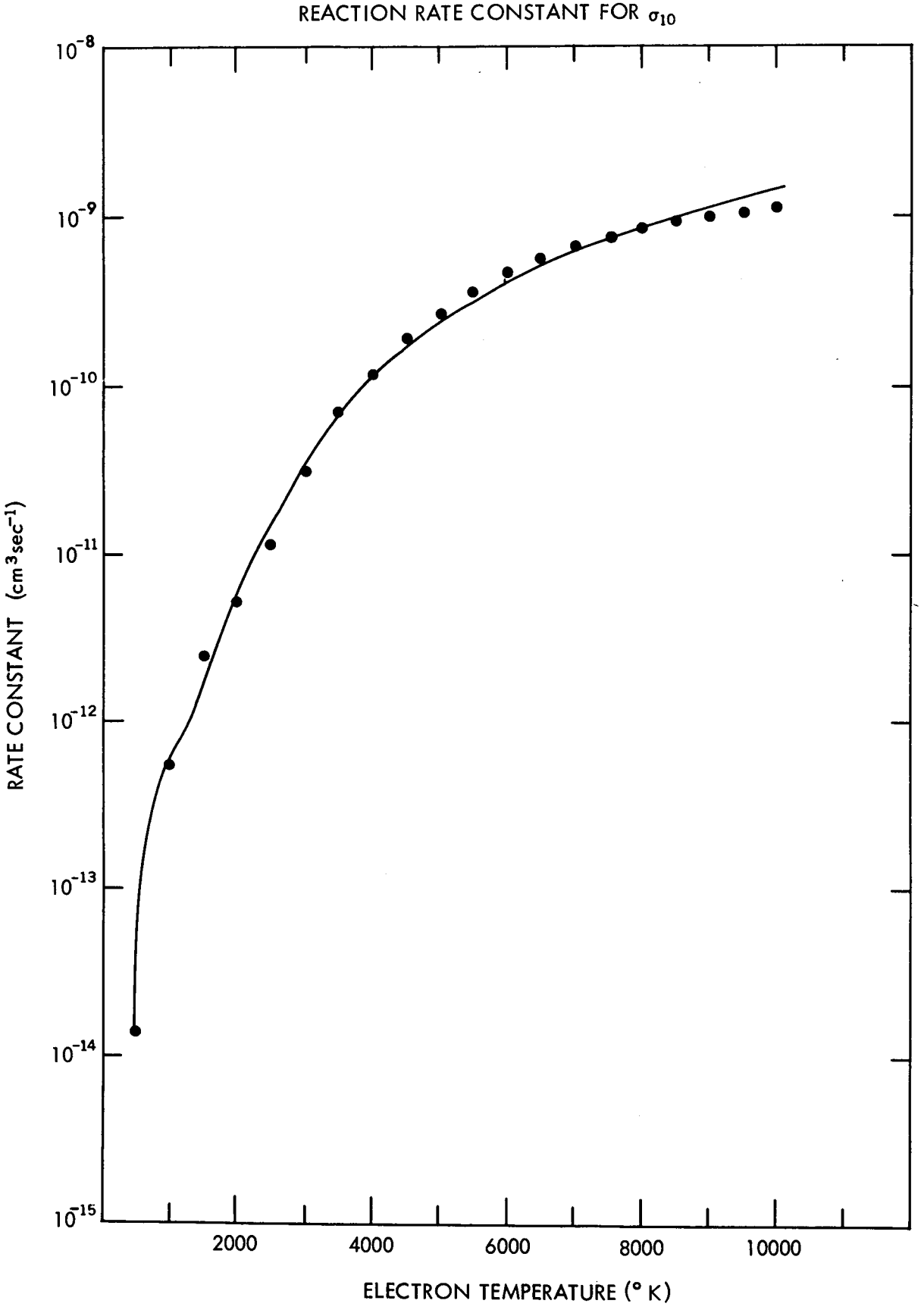

Figure A1-1. Reaction rate constant calculated from σ_{10}

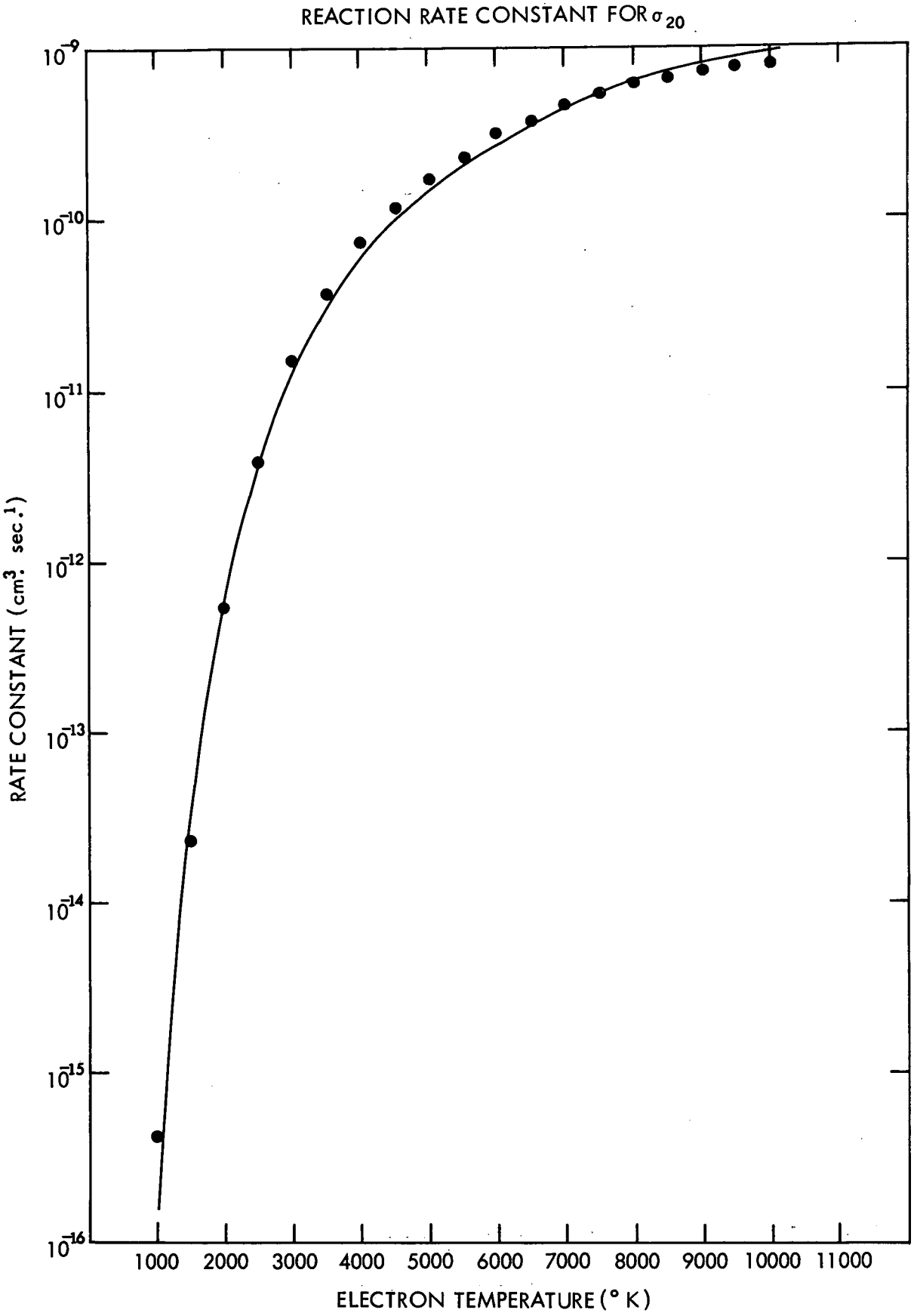

Figure A1-2. Reaction rate constant calculated from σ_{20}

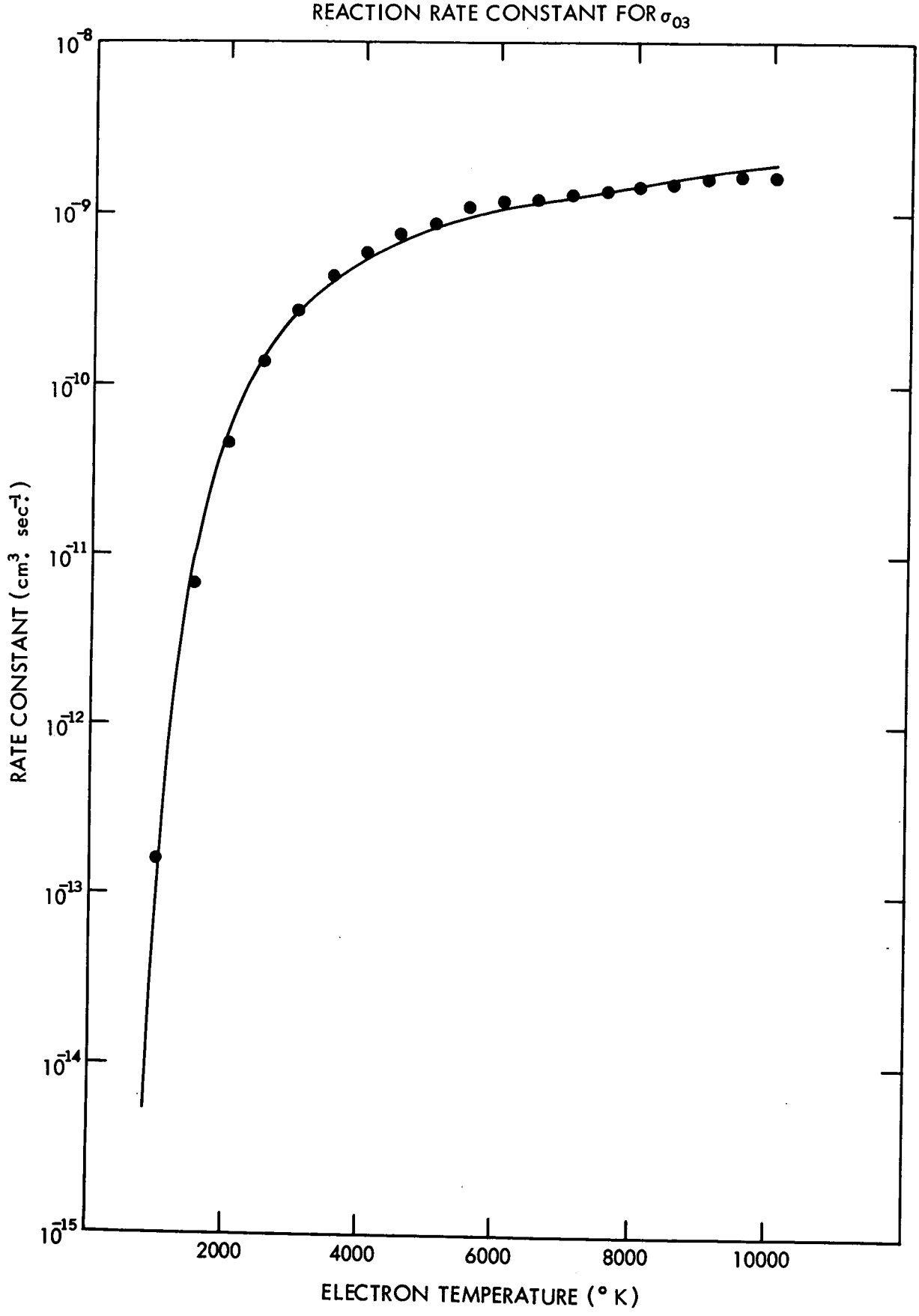

Figure A1-3. Reaction rate constant calculated from σ_{03}

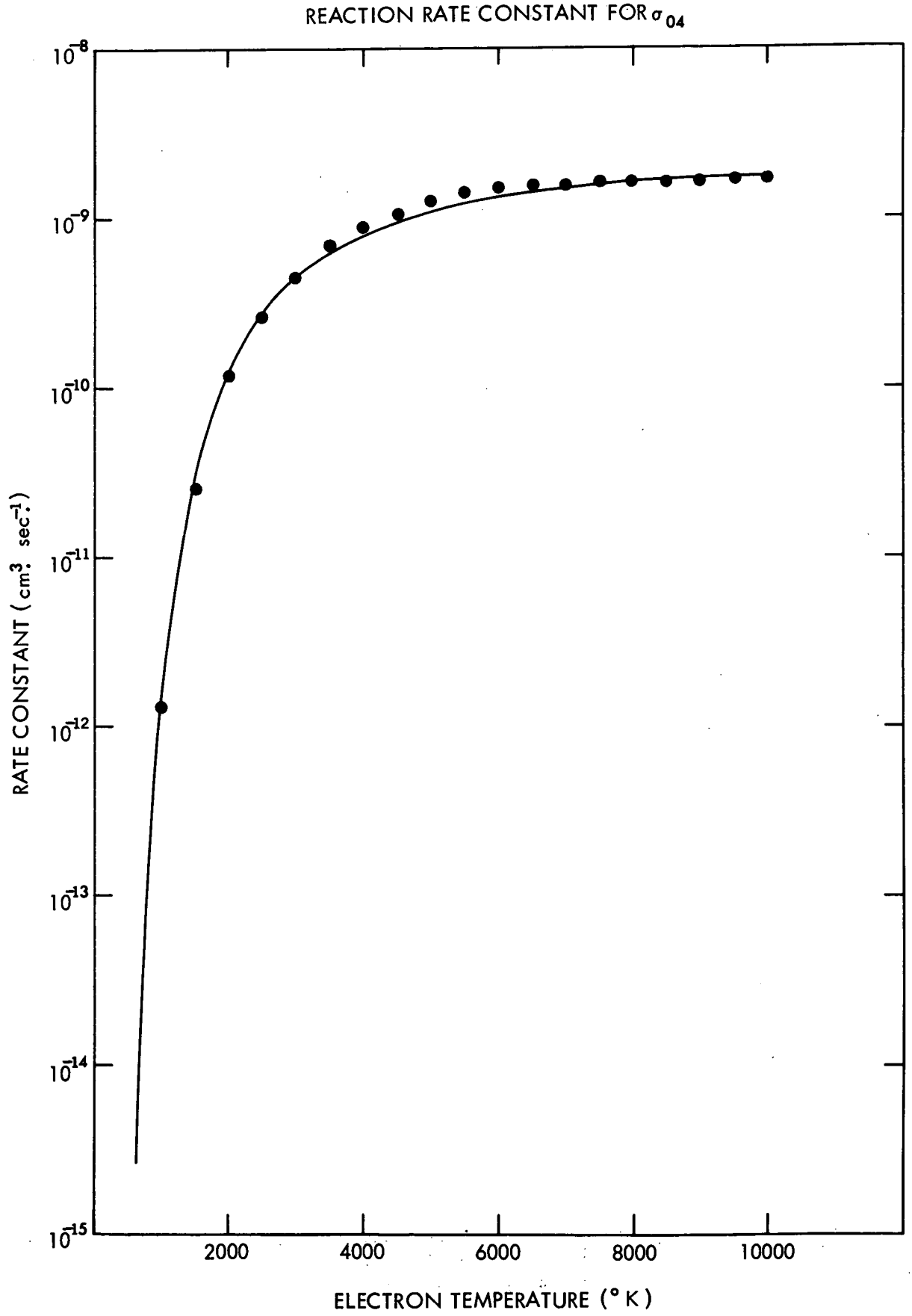

Figure A1-4. Reaction rate constant calculated from σ_{04}

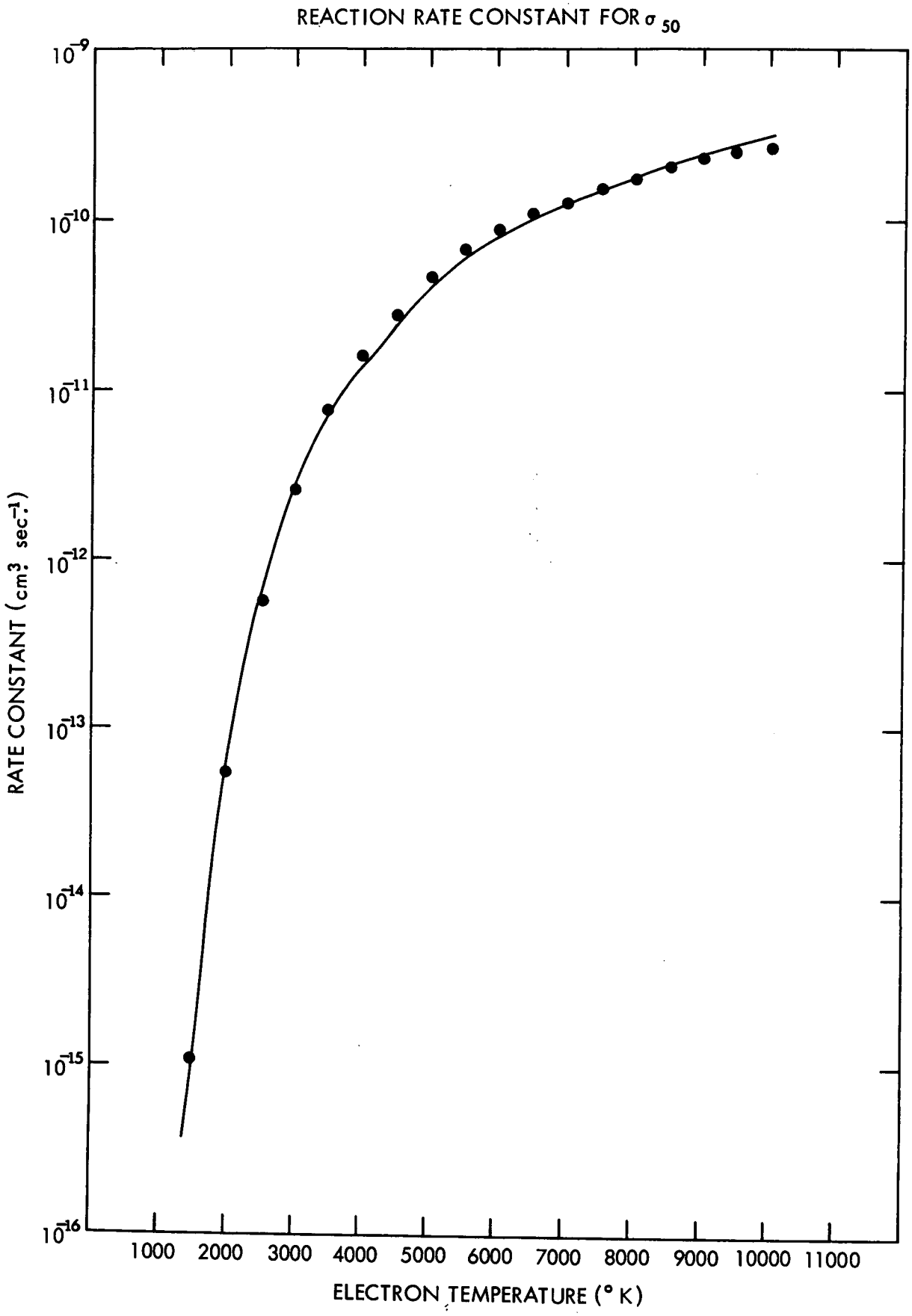

Figure A1-5. Reaction rate constant calculated from σ_{50}

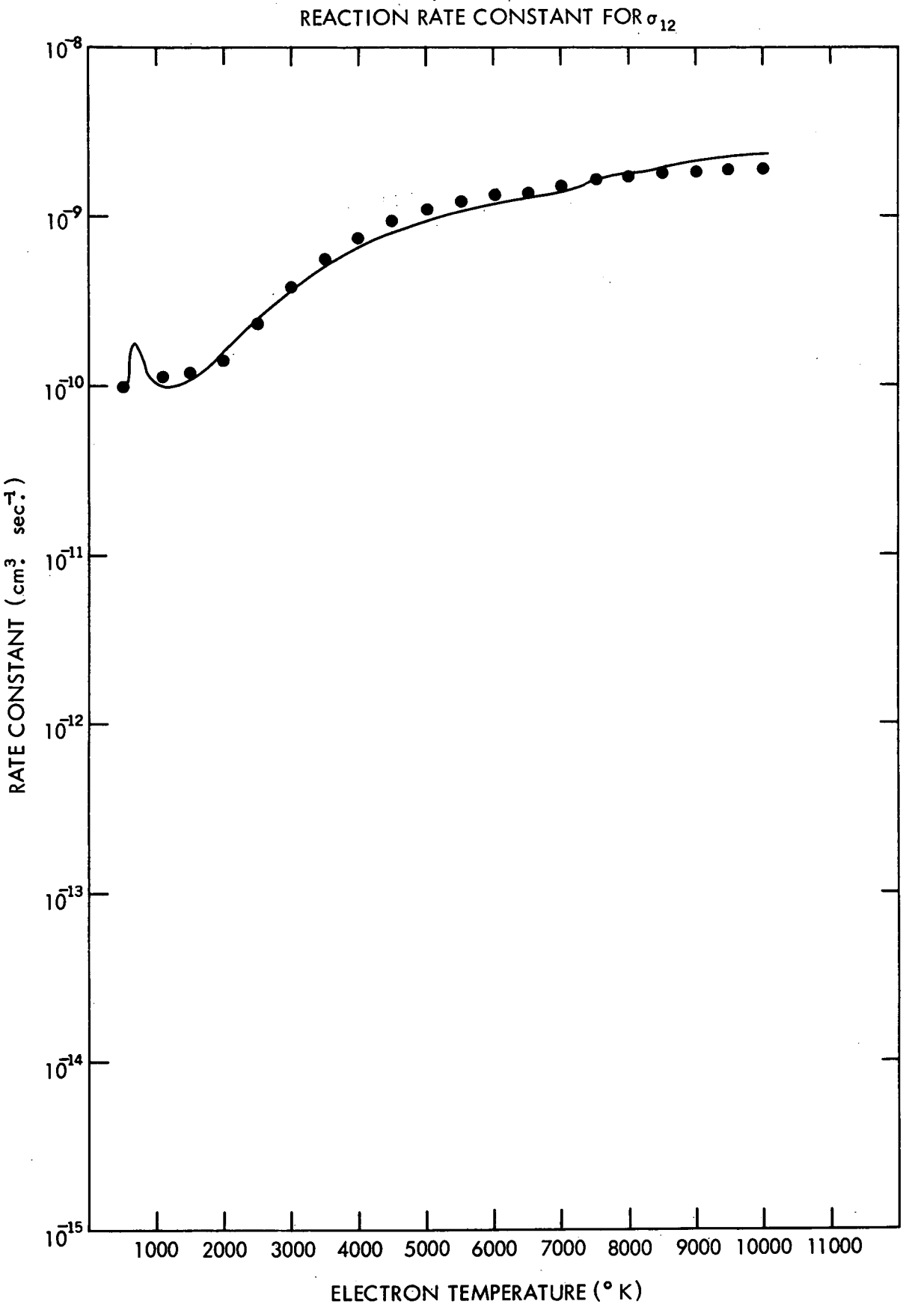

Figure A1-6. Reaction rate constant calculated from σ_{12}

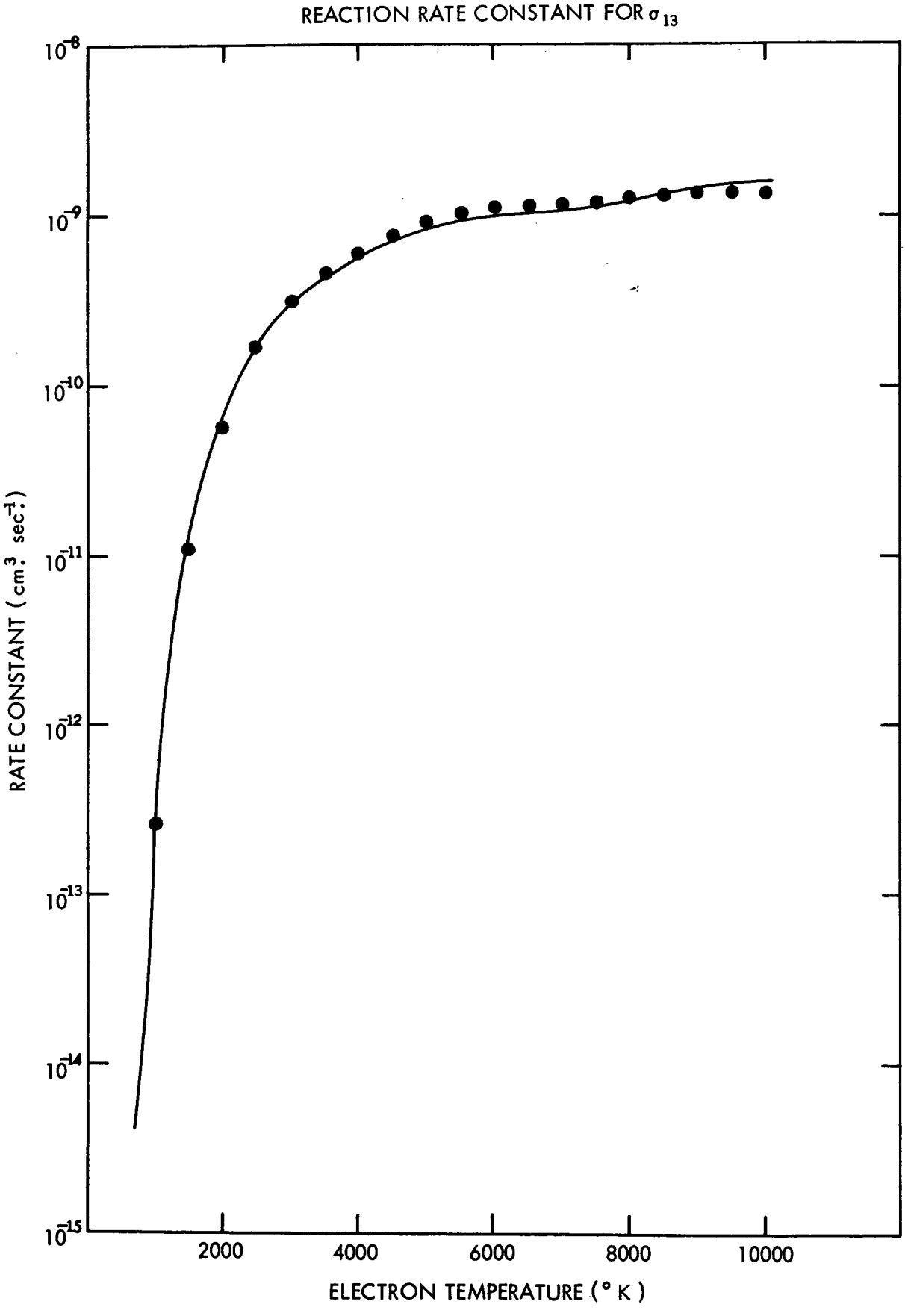

Figure A1-7. Reaction rate constant calculated from σ_{13}

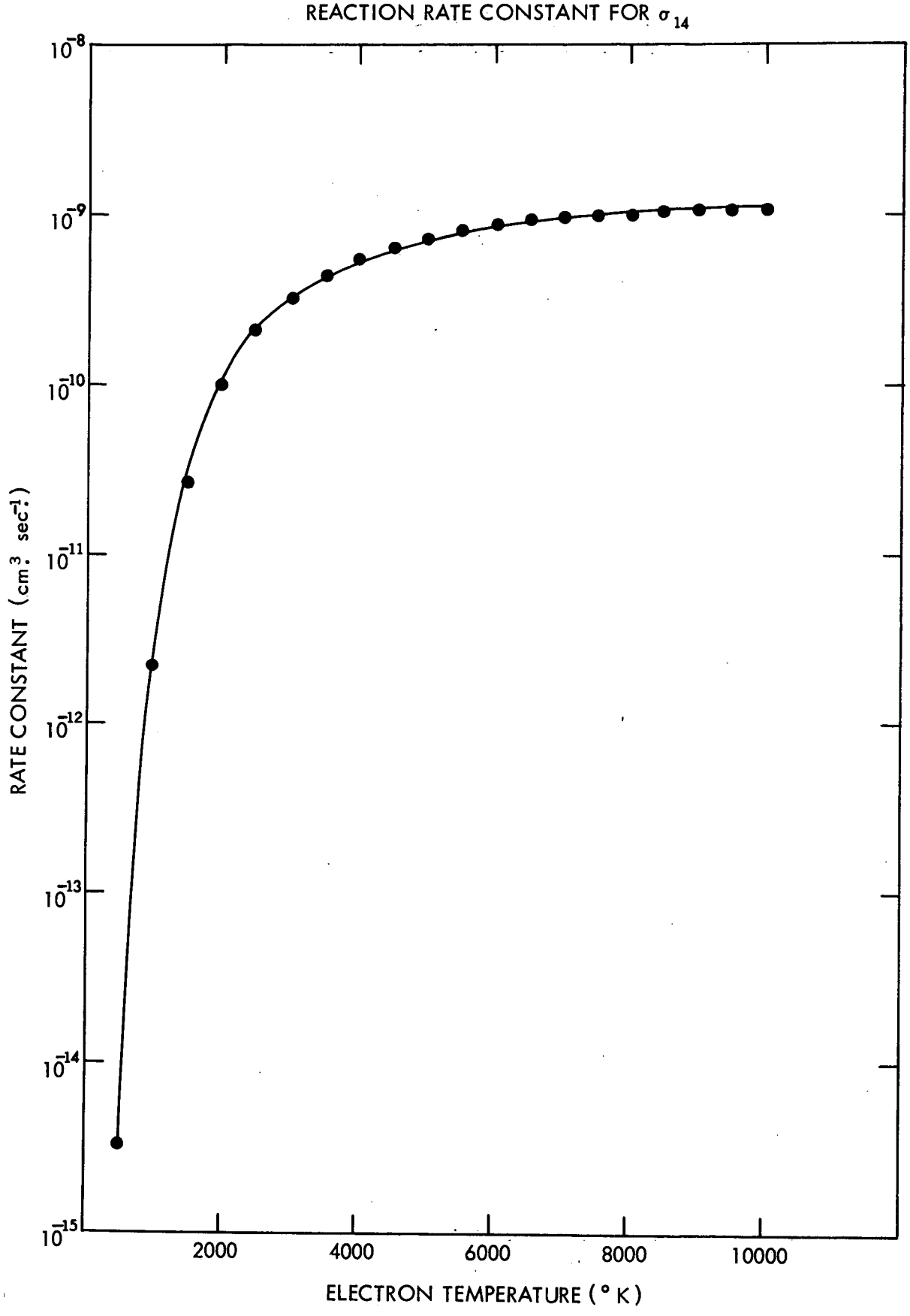

Figure A1-8. Reaction rate constant calculated from σ_{14}

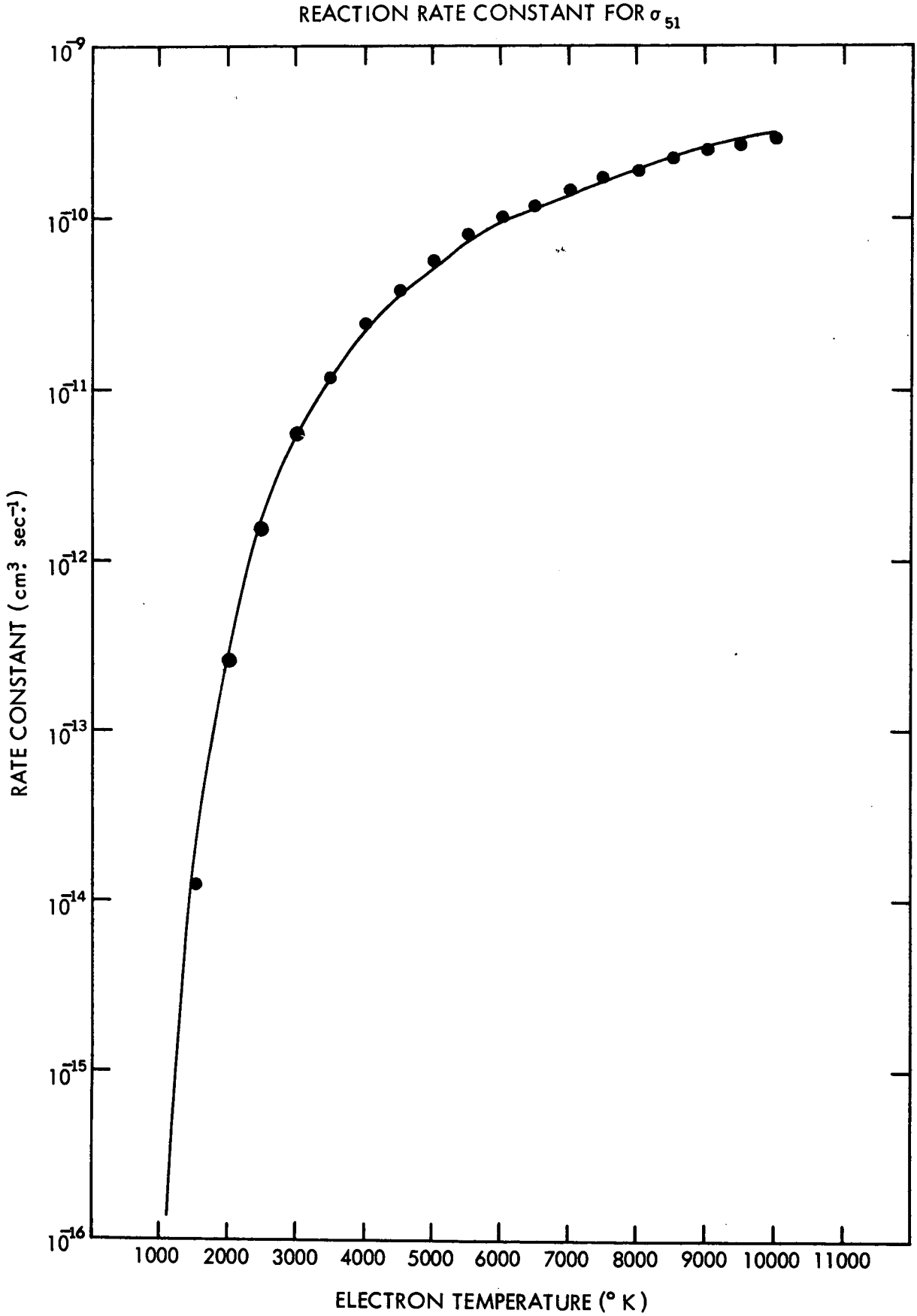

Figure A1-9. Reaction rate constant calculated from σ_{51}

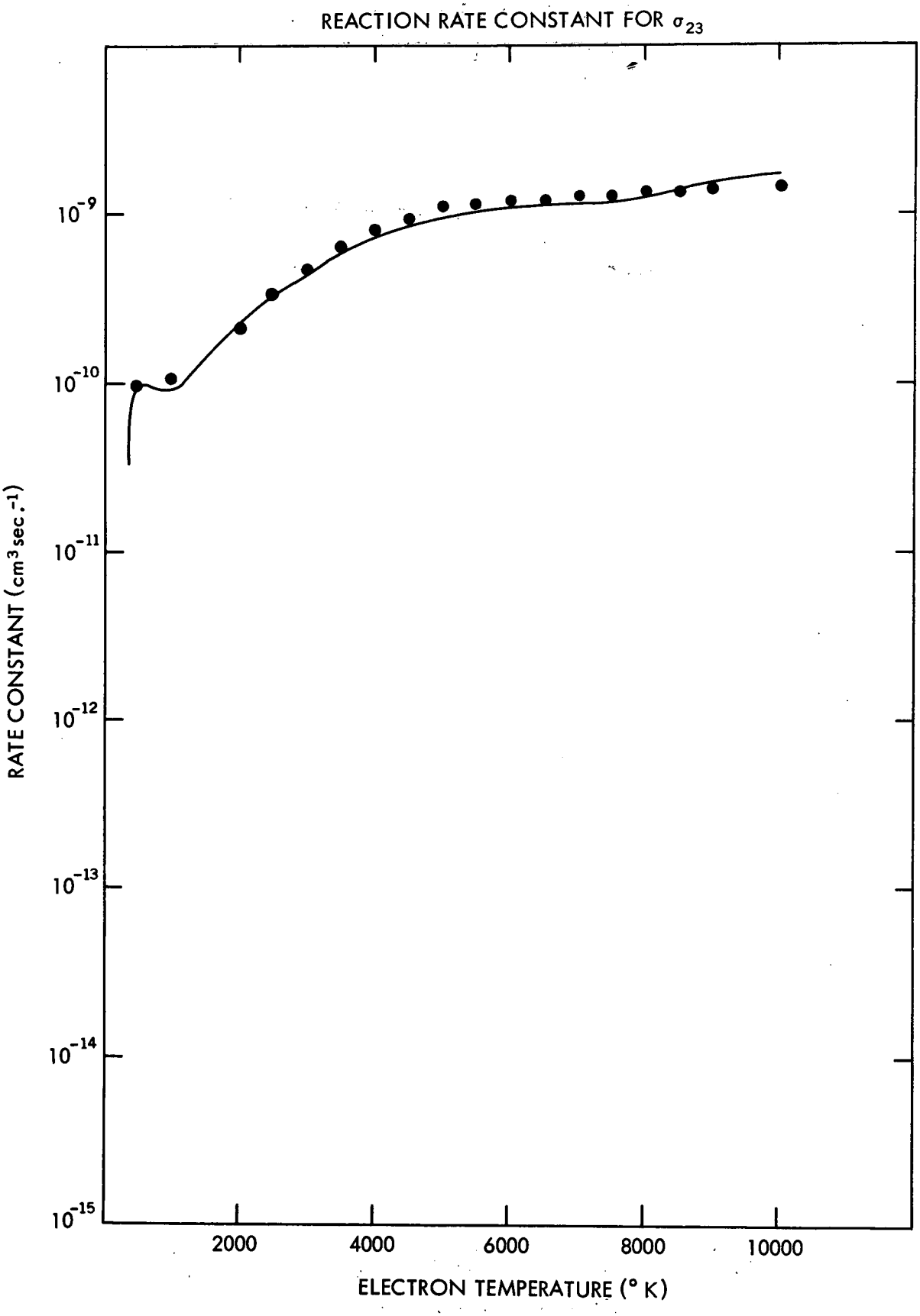

Figure A1-10. Reaction rate constant calculated from σ_{23}

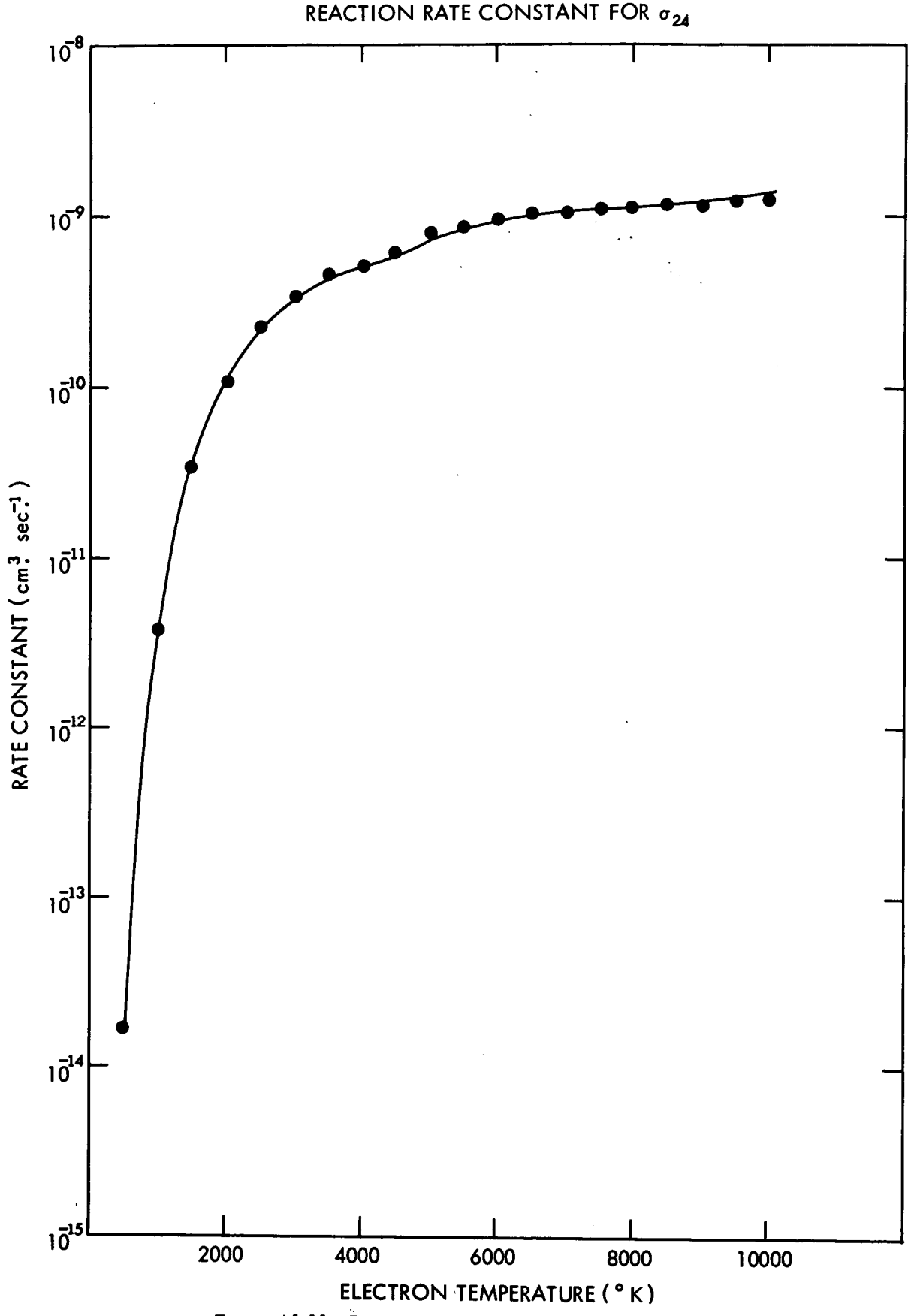

Figure A1-11. Reaction rate constant calculated from σ_{24}

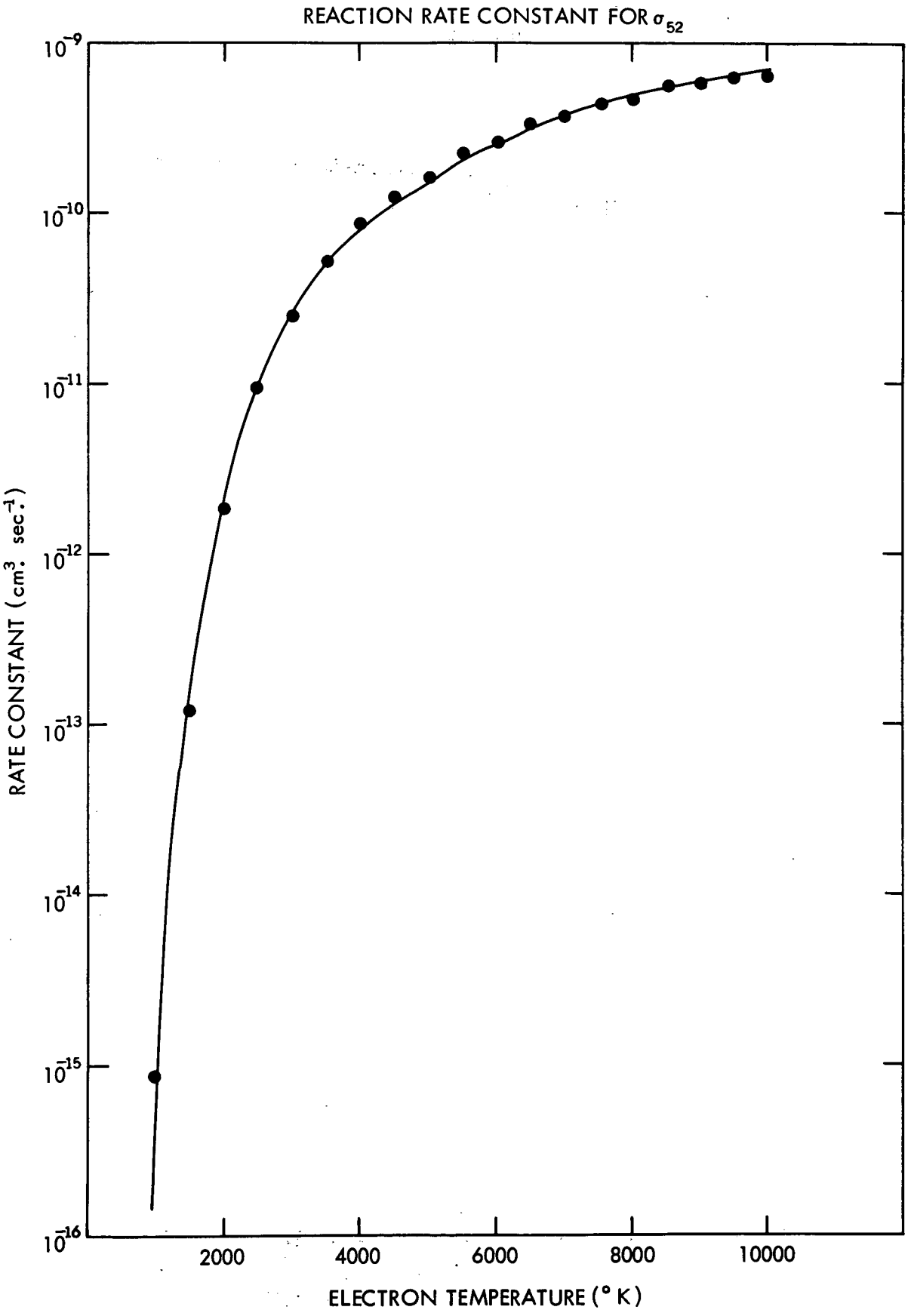

Figure A1-12. Reaction rate constant calculated from σ_{52}

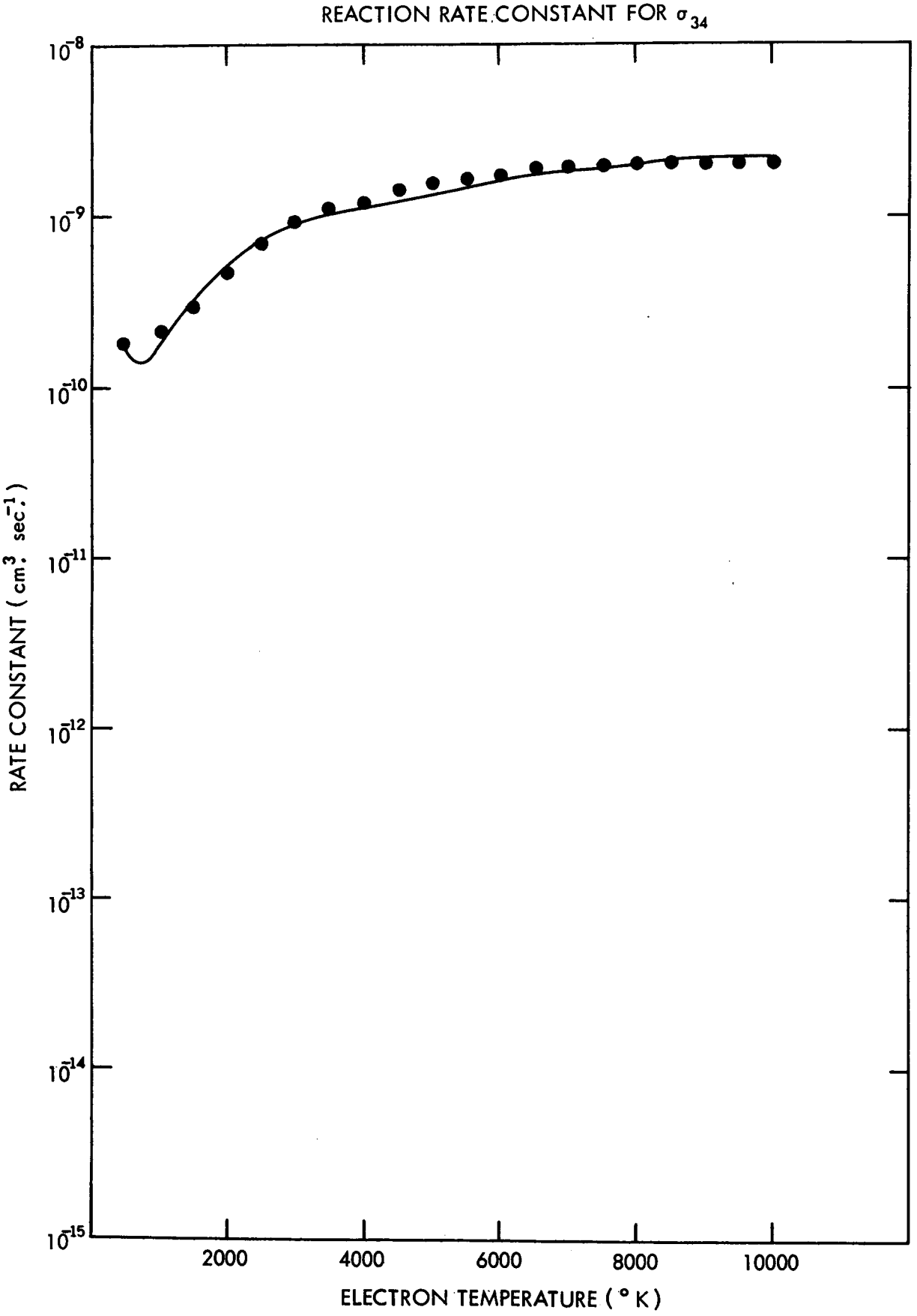

Figure A1-13. Reaction rate constant calculated from σ_{34}

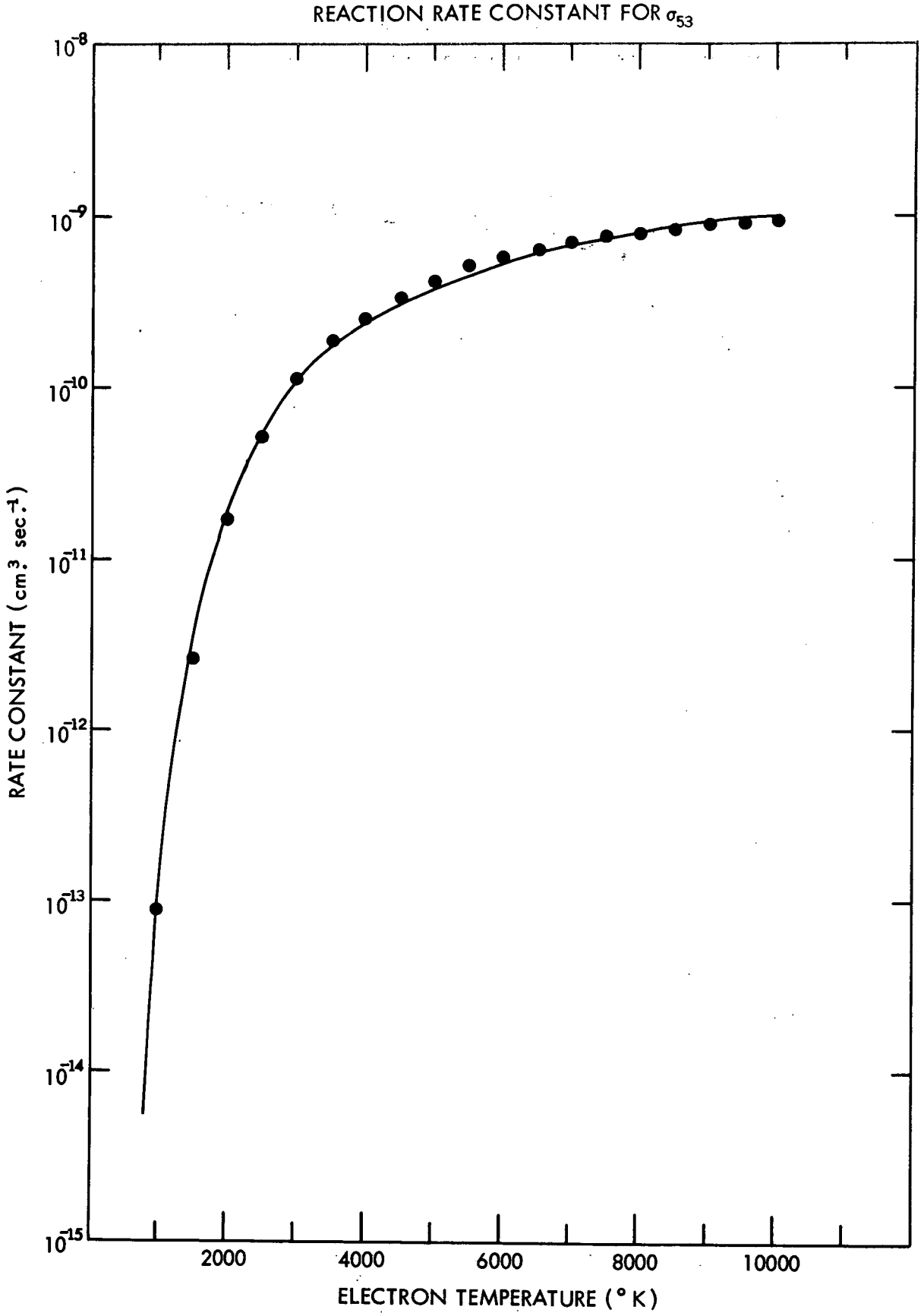

Figure A1-14. Reaction rate constant calculated from σ_{53}

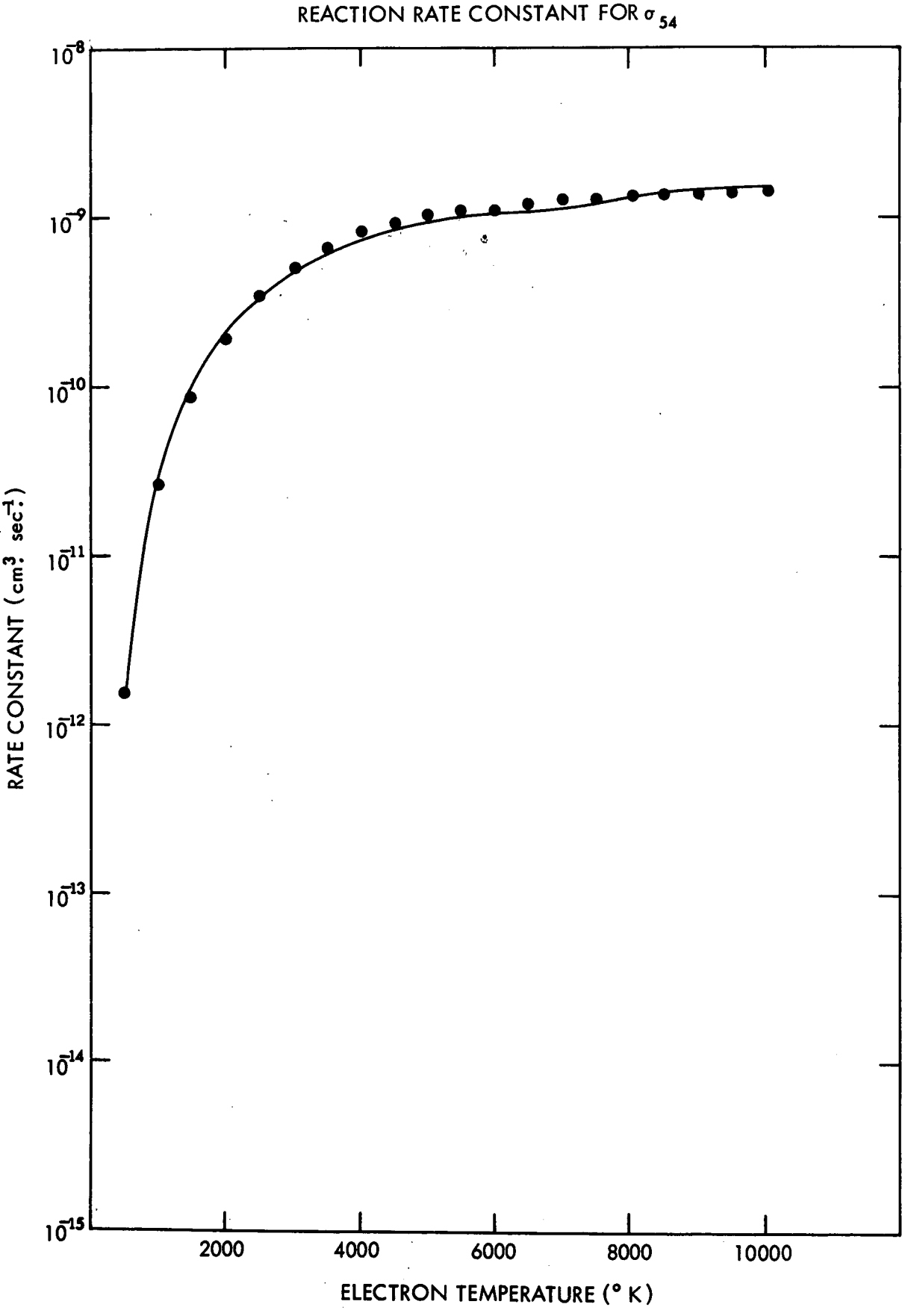

Figure A1-15. Reaction rate constant calculated from σ_{54}

It was found that the reaction rates could be adequately reproduced by a four parameter function of the electron temperature of the form

$$I_{ij} = \text{Exp}\left(P_1 + \frac{P_2}{T_e} + \frac{P_3}{T_e^2} + \frac{P_4}{T_e^3}\right) \qquad \text{(A1-22)}$$

The four parameters for each cross section of Table (1) are given in Table (2). Equation (A1-22) reproduces the integrated cross section results, over the electron temperature range, to better than 40% in all cases. This was considered acceptable considering the order of magnitude accuracy of the basic cross section calculations. The reaction rates from (A1-22) are also plotted as lines in Figures A1-1 through A1-15. Equations (A1-22) and (A1-21) were used to calculate the reaction rates used in further calculations.

APPENDIX II

SIMPLIFICATION OF THE CONTINUITY EQUATIONS

From section 2.4 we have for the continuity equation of the number of N_2^* in level i

$$\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial z}(\vec{F}_i)_z = \sum_{j=0} \{A_{ij}\, n_j - A_{ji}\, n_i\}$$

$$+ P_{1,0:0,1}\, \nu i \sum_{j=0} (j+1)\,[n_{i-1}\, n_{j+1} - n_i\, n_j]$$

$$+ P_{1,0:0,1}\, \nu\, (i+1) \sum_{j=1} j\,[n_{i+1}\, n_{j-1} - n_i\, n_j]$$

$$+ C_{1,0}\, \nu'\, n\,[0]\,[i\, n_{i-1} + (i+1)\, e^{\theta/T} n_{i+1}$$

$$+ (i\, e^{\theta/T} + i + 1)\, n_i] \qquad (2\text{-}22)$$

These are a set of 6 coupled, non-linear, partial differential equations. The coefficients are functions of altitude through the altitudinal dependence of the model atmosphere and ionosphere parameters.

Each solution to equations (2-22) will be written as a sum of a Boltzmann distributed density, n_i, and a remainder term, ϵ_i, to simplify the coupling between the equations. Thus,

$$n_i = n_i' + \epsilon_i \qquad (A2\text{-}1)$$

and we require that

$$\sum_{i=0} i\, n_i = \sum_{i=0} i\, n_i' \qquad (A2\text{-}2)$$

$$\sum_{i=0} n_i = \sum_{i=0} n_i' = n \tag{A2-3}$$

Equation (A2-2) and (A2-3), respectively, require the vibrational energy and density of the Maxwell-Boltzmann distributed density to be the energy and density of the solution for the set of equations (2-22). Thus, from equation (A2-1) we have using (A2-2) and (A2-3)

$$\sum_{i=0} i\,\epsilon_i = 0 \tag{A2-4}$$

$$\sum_{i=0} \epsilon_i = 0 \tag{A2-5}$$

Substituting (A2-1) into the flux term (A2-21) we obtain

$$\vec{F}_i = \vec{F}_i' + \vec{\mathfrak{I}}_i \tag{A2-6}$$

where

$$\vec{F}_i' = -D\left[\nabla n_i' + \frac{n_i'}{H}\hat{k}\right] \tag{A2-7}$$

$$\vec{\mathfrak{I}}_i' = -D\left[\nabla \epsilon_i + \frac{\epsilon_i}{H}\hat{k}\right] \tag{A2-8}$$

Substituting (A2-1) into (2-22) and rearranging terms we have

$$\frac{\partial n_i'}{\partial t} + \frac{\partial}{\partial z}(\vec{F}_i')_z + \frac{\partial \epsilon_i}{\partial t} + \frac{\partial}{\partial z}(\vec{\mathfrak{I}}_i)_z = \sum_{j=0} \{A_{ij}(n_j' + \epsilon_j)$$

$$- A_{ji}(n_i' + \epsilon_i)\} + P_{1,0:0,1}\,\nu\, i \sum_{j=0} (j+1)\,[n_{i-1}'\, n_{j+1}'$$

$$- n_i' n_j' + \epsilon_{i-1} n_{j+1}' + \epsilon_{j+1} n_{i-1}' - \epsilon_i n_j'$$

$$- \epsilon_j n_i' + \epsilon_{i-1} \epsilon_{j+1} - \epsilon_i \epsilon_j]$$

$$+ P_{1,0:0,1} \nu (i + 1) \sum_{j=1} j [n_{i+1}' n_{j-1}' - n_i' n_j'$$

$$+ \epsilon_{i+1} n_{j-1}' + \epsilon_{j-1} n_{i+1}' - \epsilon_i n_j' - \epsilon_j n' i$$

$$+ \epsilon_{i+1} \epsilon_{j-1} - \epsilon_j \epsilon_j] + C_{1,0} \nu' n[0] \quad [i (n_{i-1}' + \epsilon_{i-1})$$

$$+ (i + 1) e^{\theta/T} (n_{i+1}' + \epsilon_{i+1}) - (i e^{\theta/T} + i + 1) (n' _i + \epsilon_i)] \quad \textbf{(A2-9)}$$

We have

$$n_{i-1}' n_{j+1}' - n_i' n_j' = n_{i+1}' n_{j-1}' - n_i' n_j' \quad \textbf{(A2-10)}$$

Using (A2-10) in (A2-9) and rearranging terms we have

$$\frac{\partial n_i'}{\partial t} + \frac{\partial}{\partial z} (\vec{F}_i')_z + \frac{\partial \epsilon_i}{\partial t} + \frac{\partial}{\partial z} (\vec{\mathfrak{I}}_i)_z = \sum_{j=0} \{A_{ij} (n_j' + \epsilon_j)$$

$$+ A_{ji} (n_i' + \epsilon_i)\} + P_{1,0:0,1} \nu \left[i \epsilon_{i-1} \sum_{j=0} (j + 1) n_{j+1}' \right.$$

$$- (i + 1) \epsilon_i \sum_{j=1} j n_j' + i n_{i-1}' \sum_{j=0} (j + 1) \epsilon_{j+1} - (i + 1) n_i' \sum_{j=1} j \epsilon_j$$

$$- i \epsilon_i \sum_{j=0} (j + 1) n_j' + (i + 1) \epsilon_{i+1} \sum_{j=1} j n_{j-1}' - i n_i' \sum_{j=0} (j + 1) \epsilon_j$$

$$+ (i+1)\, n'_{i+1} \sum_{j=0} j\, \epsilon_{j-1} + i\, \epsilon_{i-1} \sum_{j=0} (j+1)\, \epsilon_{j+1}$$

$$- (i+1)\, \epsilon_i \sum_{j=1} j\, \epsilon_j - i\, \epsilon_i \sum_{j=0} (j+1)\, \epsilon_j + (i+1)\, \epsilon_{i+1} \sum_{j=1} j\, \epsilon_{j-1} \qquad \text{(A2-11)}$$

$$+ C_{1,0}\, \nu'\, n\,[0]\, [i\,(n'_{i-1} + \epsilon_{i-1}) + (i+1)\, e^{\theta/T}\,(n_{i+1} + \epsilon_{i+1})$$

$$- (i\, e^{\theta/T} + i + 1)\,(n'_i + \epsilon_i)]$$

Using equations (A2-4) and (A2-5) in (A2-11) the 5th, 6th, 9th, 10th, 11th, 12th, 13th, and 14th terms on the right hand side are zero. Thus we have

$$\frac{\partial n'_i}{\partial t} + \frac{\partial}{\partial z}(\vec{F}'_i)_z + \frac{\partial \epsilon_i}{\partial t} + \frac{\partial}{\partial z}(\vec{\Theta}_i)_z = \sum_{j=0} \{A_{ij}\,(n'_j + \epsilon_j)$$

$$- A_{ji}\,(n'_i + \epsilon_i)\} + P_{1,0:0,1}\, \nu \left[\{i\, \epsilon_{i-1} - (i+1)\, \epsilon_i\} \sum_{j=1} j\, n'_j \right.$$

$$\left. + \{(i+1)\, \epsilon_{i+1} - i\, \epsilon_i\} \sum_{j=1} j\, n'_{j-1} \right] + C_{1,0}\, \nu'\, n\,[0]\, [i\,(n'_{i-1} + \epsilon_{i-1})$$

$$+ (i+1)\, e^{\theta/T}\,(n'_{i+1} + \epsilon_{i+1}) - (i\, e^{\theta/T} + i + 1)$$

$$(n'_i + \epsilon_i)] \qquad \text{(A2-12)}$$

A.2.1 The equation for the Boltzmann part of the solution.

Multiply (A2-12) by i and sum over i to get

$$\frac{\partial}{\partial t}\sum_{i=0} i\, n_i' = \frac{\partial}{\partial z}\left(\sum_{i=0} i\, \vec{F}_i'\right)_z = \sum_{i=0}\sum_{j=0} i\,\{A_{ij}\,(n_j' + \epsilon_j)$$

$$- A_{ji}\,(n_i' + \epsilon_i)\} + P_{1,0:0,1}\,\nu\left[\sum_{j=1} j\, n_j'\left\{\sum_{i=0}\left[i^2\,\epsilon_{i-1}\right.\right.\right.$$

$$\left.\left.\left. - (i+1)\,\epsilon_i\right]\right\} + \sum_{j=1} j\, n_{j-1}'\left\{\sum_{i=0}\left[i\,(i+1)\,\epsilon_{i+1} - i^2\,\epsilon_i\right]\right\}\right] \qquad \text{(A2-13)}$$

$$+ C_{1,0}\,\nu'\, n\,[0]\left[\sum_{i=0}\{i^2\, n_{i-1}' + i\,(i+1)\, e^{\theta/T}\, n_{i+1}'\right.$$

$$\left. - i\,(i\, e^{\theta/T} + i + 1)\, n_i'\right\} + \sum_{i=0}\{i^2\,\epsilon_{i-1} - i\,(i+1)\,\epsilon_i\}$$

$$\left. + e^{\theta/T}\sum_{i=0}\{i\,(i+1)\,\epsilon_{i+1} - i^2\,\epsilon_i\}\right]$$

where we have used (A2-4) and

$$\sum_{i=0} i\,\vec{\mathfrak{J}}_i = -\sum_{i=0} i\, D\left[\nabla\epsilon_i + \frac{\epsilon_i}{H}\hat{k}\right]$$

$$= -D\left[\nabla\sum_{i=0} i\,\epsilon_i + \sum_{i=0} i\,\frac{\epsilon_i}{H}\hat{k}\right]$$

$$= 0 \qquad \text{(A2-14)}$$

Consider

$$\sum_{i=0}\left[i^2\,\epsilon_{i-1} - i\,(i+1)\,\epsilon_i\right] = \sum_{i=1} i^2\,\epsilon_{i-1} - \sum_{i=0} i^2\,\epsilon_i - \sum_{i=0} i\,\epsilon_i$$

$$= \sum_{i=0}(i+1)^2\,\epsilon_i - \sum_{i=0} i^2\,\epsilon_i$$

$$= \sum_{i=0} (2\,i + 1)\,\epsilon_i \qquad \text{(A2-15)}$$

$$= 0$$

Also consider

$$\sum_{i=0} [i\,(i+1)\,\epsilon_{i+1} - i^2\,\epsilon_i] = \sum_{i=0} i\,(i-1)\,\epsilon_i - \sum_{i=0} i^2\,\epsilon_i$$

$$= -\sum_{i=0} i\,\epsilon_i$$

$$= 0 \qquad \text{(A2-16)}$$

Using (A2-15) and (A2-16) in (A2-13) we have

$$\frac{\partial}{\partial t}\sum_{i=0} i\,n_i' + \frac{\partial}{\partial z}\left(\sum_{i=0} i\,\vec{F}_i'\right)_z = \sum_{i=0}\sum_{j=0} i\{A_{ij}\,(n_j' + \epsilon_j)$$

$$- A_{ji}\,(n_i' + \epsilon_i)\} + C_{1,0}\,\nu'\,[0]\sum_{i=0}\{i^2\,n_{i-1}' \qquad \text{(A2-17)}$$

$$+ i\,(i+1)\,e^{\theta/T}\,n_{i+1}' - i\,(i\,e^{\theta/T} + i + 1)\,n_i'\}$$

Consider

$$\sum_{i=0}\{i^2\,n_{i-1}' + i\,(i+1)\,e^{\theta/T}\,n_{i+1}' - i\,(i\,e^{\theta/T} + i + 1)\,n_i'\}$$

$$= \sum_{i=0}\{(i+1)^2\,n_i' - i^2\,n_i' - i\,n_i' + e^{\theta/T}\,\{i\,(i-1)\,n_i' - i^2\,n_i'\}\}$$

$$= \sum_{i=0} \{(i+1) - i\, e^{\theta/T}\}\, n_i' \qquad \text{(A2-18)}$$

Therefore equation (A2-17) becomes

$$\frac{\partial}{\partial t}\sum_{i=0} i\, n_i' + \frac{\partial}{\partial z}\left(\sum_{i=0} i\, \vec{F}_i'\right)_z = \sum_{i=0}\sum_{j=0} i\{A_{ij}\,(n_j' + \epsilon_j) - A_{ji}\,(n_i' + \epsilon_i)\} + C_{1,0}\,\nu'\, n\,[0]\left[\sum_{i=0}(i+1)\, n_i' - e^{\theta/T}\sum_{i=0} i\, n_i'\right] \qquad \text{(A2-19)}$$

Let Z_p be the partition function for the Boltzmann distributed part of the solution. Then,

$$Z_p = \frac{1}{1 - e^{-\alpha}} \qquad \text{(A2-20)}$$

where

$$\alpha = \frac{\theta}{T_v} \qquad \text{(A2-21)}$$

and T_v is the vibrational temperature. Therefore

$$\sum_{i=0} i\, n_i' = \sum_{i=0} i\, \frac{n}{Z_p}\, e^{-\alpha} = \frac{n}{Z_p}\,\frac{e^{-\alpha}}{(1 - e^{-\alpha})^2}$$

$$= n\,(Z_p - 1) \qquad \text{(A2-23)}$$

Also

$$\sum_{i=0} i \vec{F}_i = - D \left[\nabla \sum_{i=0} i\, n_i' + \sum_{i=0} i \frac{n_i'}{H} \hat{k} \right]$$

$$= - D \left[\nabla n (Z_p - 1) + \frac{n (Z_p - 1)}{H} \hat{k} \right] \qquad \text{(A2-24)}$$

Consider

$$\sum_{i=0} i \sum_{j=0} \{A_{ij} (n_j' + \epsilon_j) - A_{ji} (n_i' + \epsilon_i)\} = (n_0' + \epsilon_0) \left\{ \sum_{i=0} i\, A_{i0} (1 - \delta_{i0}) \right\}$$

$$+ (n_1' + \epsilon_1) \left\{ \sum_{i=0} i\, A_{i1} (1 - \delta_{i1}) - \sum_{j=0} A_{j1} (1 - \delta_{1j}) \right\}$$

$$+ (n_2' + \epsilon_2) \left\{ \sum_{i=0} i\, A_{i2} (1 - \delta_{i2}) - \sum_{j=0} 2\, A_{j2} (1 - \delta_{j2}) \right\}$$

$$+ \ldots$$

$$+ (n_k' + \epsilon_k) \left\{ \sum_{i=0} i\, A_{ik} (1 - \delta_{ik}) - \sum_{j=0} k\, A_{jk} (1 - \delta_{jk}) \right\}$$

$$+ \ldots$$

$$= (n_0' + \epsilon_0) \left\{ \sum_{i=0} i (1 - \delta_{i0})\, A_{i0} + (n_1' + \epsilon_1) \sum_{i=0} (i - 1)\, A_{i1} \right\}$$

$$+ (n_2' + \epsilon_2) \left\{ \sum_{i=0} (i - 2)\, A_{j2} \right\} + \ldots$$

$$+ (n_k' + \epsilon_k) \left\{ \sum_{i=0} (i - k)\, A_{jk} \right\} + \ldots$$

$$= \sum_{i=0} \sum_{j=0} (n_j' + \epsilon_j) (i - j)\, A_{ij} \qquad \text{(A2-25)}$$

Using (A2-23), (A2-24) and (A2-25) in equation (A2-19) we have

$$\frac{\partial}{\partial t} n (Z_p - 1) + \frac{\partial}{\partial z} \left\{ - D \left[\frac{\partial}{\partial z} n (Z_p - 1) + \frac{n (Z_p - 1)}{H} \right] \right\}$$

$$= \sum_{i=0} \sum_{j=0} (n_j' + \epsilon_j) (i - j) A_{ij}$$

$$+ C_{1,0} \nu' n [0] [n (Z_p - 1) + n - e^{\theta/T} n (Z_p - 1)] \quad \text{(A2-26)}$$

Let

$$\psi = (Z_p - 1) \quad \text{(A2-27)}$$

and use

$$\frac{\partial n}{\partial t} = 0$$

and

$$(Z_p - 1) \frac{\partial n}{\partial z} = - \frac{n (Z_p - 1)}{H}$$

in equation (A2-26) to obtain

$$n \frac{\partial \psi}{\partial t} + \frac{\partial}{\partial z} \left(- D n \frac{\partial \psi}{\partial z} \right) = \sum_{i=0} \sum_{j=0} (n_j' + \epsilon_j) (i - j) A_{ij}$$

$$+ C_{1,0} \nu' n [0] n [\psi + 1 - e^{\theta/T} \psi] \quad \text{(A2-28)}$$

Using

$$n_j' = \frac{n}{Z_p} (e^{-\alpha})^j$$

$$= \frac{n}{\psi + 1} \left(\frac{\psi}{\psi + 1} \right)^j \quad \text{(A2-29)}$$

and dividing equation (A2-28) by n we have

$$\frac{\partial \psi}{\partial t} - \frac{1}{n}\left(\frac{\partial D n}{\partial z}\right)\frac{\partial \psi}{\partial z} - D\frac{\partial \psi^2}{\partial z^2} = \sum_{i=0}\sum_{j=0}\left[\frac{1}{\psi+1}\left(\frac{\psi}{\psi+1}\right)^j + \frac{\epsilon_j}{n}\right]$$

$$(i-j)\,A_{ij} + C_{1,0}\,\nu' n\,[0]\cdot[\psi + 1 - e^{\theta/T}\psi] \qquad \text{(A2-30)}$$

The boundary conditions become for: set 1;

initial condition: $\psi(z, 0) = 0$

lower boundary: $\psi(120, t) = 0$

upper boundary: $\frac{\partial n_i}{\partial z} = -\frac{n_i}{H} \Rightarrow \frac{\partial n_i'}{\partial z} + \frac{\partial \epsilon_i}{\partial z} = -\frac{n_i'}{H} - \frac{\epsilon_i}{H}$

Using (A2-23)

$$\frac{\partial}{\partial z}\sum_{i=p} i\, n_i' = -\sum_{i=0} i\frac{n_i'}{H}$$

Using (A2-23) and (A2-27) we have

$$\frac{\partial}{\partial z} n\psi \Big|_{z=\infty} = -\frac{n\psi}{H}\Big|_{z=\infty} \qquad \text{(A2-31)}$$

Thus,

$$\frac{\partial \psi}{\partial z}\Big|_{z=0} = 0$$

set 2;

initial condition: $\psi(z, 0) = \dfrac{e^{-\theta/355}}{1 - e^{-\theta/355}}$

$= 7.329241 \times 10^{-5}$

lower boundary: $\psi(0, t) = 7.329241 \times 10^{-5}$

upper boundary: $\frac{\partial \psi}{\partial z} = 0$ (A2-32)

It is worthy of note that the only coupling between equation (A2-30) and the other equations is through the ϵ_j / n term of the source of N_2^* due to electron collisions. This fact, and the expectation that ϵ_j / n is small with respect to 1 for all j of interest, will be exploited in the solution of (A2-30).

A2.2 The equations for the deviation parts of the solution.

Returning to equation (A2-12) for the ϵ_i's and treating the n_j''s as known quantities we have

$$\frac{\partial}{\partial t}\epsilon_i + \frac{\partial}{\partial z}(\vec{\Im}_i)_z = \sum_{j=0}\{A_{ij}(n_j' + \epsilon_j) - A_{ji}(n_i' + \epsilon_i)\} - \frac{\partial n_i'}{\partial t}$$

$$- \frac{\partial}{\partial z}(\vec{F}_i')_z + P_{1,0:0,1}\,\nu\left[\{i\,\epsilon_{i-1} - (i+1)\,\epsilon_i\}\sum_{j=1} j\,n_j\right.$$

$$\left. + \{(i+1)\,\epsilon_{i+1} - i\,\epsilon_i\}\sum_{j=1} j\,n_{j-1}'\right] + C_{1,0}\,\nu'\,n\,[0]\,[i\,(n_{i-1}'$$

$$+ \epsilon_{i-1}) + (i+1)\,e^{\theta/T}(n_{i+1}' + \epsilon_{i+1}) - (i\,e^{\theta/T} + i + 1)$$

$$\cdot\,(n_i' + \epsilon_i)] \qquad \text{(A2-33)}$$

Using equations (A2-23) and (A2-27) we have

$$\frac{\partial}{\partial t}\epsilon_i + \frac{\partial}{\partial z}(\vec{\Im}_i)_z = \sum_{j=0}\{A_{ij}(n_j' + \epsilon_j) - A_{ji}(n_i' + \epsilon_i)\} - \frac{\partial n_i'}{\partial t}$$

$$- \frac{\partial}{\partial z}(\vec{F}_i')_z + P_{1,0:0,1}\,\nu\,[\{i\,\epsilon_{i-1} - (i+1)\,\epsilon_i\}\,n\,\psi$$

$$+ \{(i+1)\,\epsilon_{i+1} - i\,\epsilon_i\}\, n\,(\psi+1)]$$

$$+ c_{1,0}\,\nu'\, n\,[0]\cdot[i\,(n'_{i-1}+\epsilon_{i-1}) + (i+1)\,e^{\theta/T}\,(n'_{i+1}+\epsilon_{i+1})$$

$$- (i\,e^{\theta/T} + i + 1)\,(n'_i + \epsilon_i)] \qquad \text{(A2-34)}$$

Rearranging terms in (A2-34) and dividing by n'_i, we have

$$\frac{1}{n'_i}\frac{\partial}{\partial t}\epsilon_i + \frac{1}{n'_i}\frac{\partial}{\partial z}(\vec{\mathfrak{I}}'_i)_z = \sum_{j=0}\left\{A_{ij}\left(\frac{n''_j}{n'_i} + \frac{\epsilon_j}{n'_j}\frac{n'_j}{n'_i}\right) - A_{ji}\left(1 + \frac{\epsilon_i}{n_i}\right)\right\}$$

$$- \frac{1}{n'_i}\frac{\partial}{\partial t}n'_i - \frac{1}{n'_i}\frac{\partial}{\partial z}(\vec{F}'_i)_z - \frac{\epsilon_i}{n'_i}[P_{1,0:0,1}\,\nu\, n\,\{(2i+1)\,\psi$$

$$+ i\} + C_{1,0}\,\nu'\, n\,[0]\cdot(i\,e^{\theta/T} + i + 1)]$$

$$+ \frac{\epsilon_{i-1}}{n'_{i-1}}\frac{n'_{i-1}}{n'_i}[P_{1,0:0,1}\,\nu\, i\, n\,\psi + C_{1,0}\,\nu'\, n\,[0]\cdot i]$$

$$+ \frac{\epsilon_{i+1}}{n'_{i+1}}\frac{n'_{i+1}}{n'_i}[P_{1,0:0,1}\,\nu\, n\,(i+1)\,(\psi+1) + C_{1,0}\,\nu'\, n\,[0]\cdot e^{\theta/T}\,(i+1)]$$

$$+ C_{1,0}\,\nu'\, n\,[0]\left[i\frac{n'_{i-1}}{n'_i} + (i+1)\,e^{\theta/T}\frac{n'_{i+1}}{n'_i} - (i\,e^{\theta/T} + i + 1)\right] \qquad \text{(A2-35)}$$

Consider

$$\frac{\partial}{\partial t}\frac{\epsilon_i}{n'_i} = \frac{1}{n'_i}\frac{\partial\,\epsilon_i}{\partial t} - \frac{\epsilon_i}{(n'_i)^2}\frac{\partial}{\partial t}n'_i$$

thus

$$\frac{1}{n'_i}\frac{\partial\,\epsilon_i}{\partial t} = \frac{\partial}{\partial t}\frac{\epsilon_i}{n'_i} + \frac{1}{n'_i}\frac{\epsilon_i}{n'_i}\frac{\partial}{\partial t}n'_i \qquad \text{(A2-36)}$$

Also

$$\nabla \frac{\epsilon_i}{n_i'} = \frac{1}{n_i'} \nabla \epsilon_i - \frac{\epsilon_i}{(n_i')^2} \nabla n_i'$$

Therefore (A2-37)

$$\nabla \epsilon_i = n_i' \nabla \frac{\epsilon_i}{n_i'} + \frac{\epsilon_i}{n_i'} \nabla n_i'$$

Therefore

$$\frac{1}{n_i'} \frac{\partial}{\partial z} (\vec{\Xi}_i)_z = \frac{1}{n_i'} \frac{\partial}{\partial z} \left[- D \left\{ \frac{\partial \epsilon_i}{\partial z} + \frac{\epsilon_i}{H} \right\} \right]$$

$$= \frac{1}{n_i'} \frac{\partial}{\partial z} \left[- D \left\{ n_i' \frac{\partial}{\partial z} \frac{\epsilon_i}{n_i'} + \frac{\epsilon_i}{n_i'} \frac{\partial n_i'}{\partial z} + \frac{\epsilon_i}{H} \right\} \right]$$

$$= \frac{1}{n_i'} \frac{\partial}{\partial z} \left[- Dn \frac{\partial}{\partial z} \frac{\epsilon_i}{n_i'} - D \frac{\epsilon_i}{n_i'} \left\{ \frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right\} \right] \quad \text{(A2-38)}$$

Let

$$\varphi_i = \frac{\epsilon_i}{n_i'} \quad \text{(A2-39)}$$

then (A2-36) and (A2-38) become, respectively,

$$\frac{1}{n_i'} \frac{\partial \epsilon_i}{\partial t} = \frac{\partial}{\partial t} \varphi_i + \frac{1}{n_i'} \varphi_i \frac{\partial}{\partial t} n_i' \quad \text{(A2-40)}$$

and

$$\frac{1}{n_i'} \frac{\partial}{\partial z} (\vec{y}_i)_z = \frac{1}{n_i'} \frac{\partial}{\partial z} \left[- Dn_i' \frac{\partial}{\partial z} \varphi_i - D\varphi_i \left\{ \frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right\} \right] \quad \text{(A2-41)}$$

Using (A2-39), (A2-40), (A2-41) in (A2-35) and rearranging terms we have

$$\frac{\partial}{\partial t} \varphi_i - D \frac{\partial^2}{\partial z^2} \varphi_i - \left[\frac{1}{n_i'} \frac{\partial}{\partial z} Dn_i' + \frac{1}{n_i'} D \left\{ \frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right\} \right] \frac{\partial \varphi_i}{\partial z}$$

$$+ \left[\frac{1}{n_i'} \frac{\partial}{\partial t} n_i' - \frac{1}{n_i'} \frac{\partial}{\partial z} \left\{ D \left(\frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right) \right\} + \sum_{j=0} A_{ji} (1 - \delta_{ij}) \right.$$

$$\left. + P_{1,0:0,1} \nu n \{(2i + 1) \psi + i\} + C_{1,0} \nu' n [0] (i e^{\theta/T} + i + 1) \right] \varphi_i$$

$$= \sum_{j=0} \left\{ A_{ij} (1 + \varphi_j) \, e^{-(j-1)\theta/T_V} - A_{ji} \right\} (1 - \delta_{ij}) - \frac{1}{n_i'} \frac{\partial n_i'}{\partial t}$$

$$- \frac{1}{n_i'} \frac{\partial}{\partial z} \left\{ - D \left(\frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right) \right\} + \varphi_{i-1} \, e^{\theta/T} \, [P_{1,0:0,1}, \, \nu n i \psi$$

$$+ C_{1,0} \, \nu' n [0] \, i] + \varphi_{i+1} \, e^{-\theta/T_V} \, [P_{1,0:0,1} \, \nu n (i + 1) (\psi + 1)$$

$$+ C_{1,0} \, \nu' n [0] \, e^{\theta/T} \, (i + 1)] + C_{1,0} \, \nu' n [0] \, \left[i \, e^{\theta/T_V} \right.$$

$$\left. + (i + 1) \, e^{\theta/T - \theta/T_V} - (i \, e^{\theta/T} + i + 1) \right] \qquad \text{(A2-42)}$$

Consider

$$\frac{1}{n_j'} \frac{\partial n_j'}{\partial y} \quad \text{where} \quad n_j' = n \frac{\psi^j}{(\psi + 1)^{j+1}}$$

$$\frac{1}{n_j'} \frac{\partial n_j'}{\partial y} = \frac{1}{n} \frac{\partial n}{\partial y} + \left\{ \frac{j}{\psi} - \frac{j + 1}{\psi + 1} \right\} \frac{\partial \psi}{\partial y} \qquad \text{(A2-43)}$$

Thus, if $y = t$

$$\frac{1}{n_j'} \frac{\partial n_j'}{\partial t} = \left(\frac{j}{\psi} - \frac{j + 1}{\psi + 1} \right) \frac{\partial \psi}{\partial t} \qquad \text{(A2-44)}$$

and if $y = z$

$$\frac{1}{n_j'} \frac{\partial n_j'}{\partial z} = - \frac{1}{H} + \left\{ \frac{j}{\psi} - \frac{j + 1}{\psi + 1} \right\} \frac{\partial \psi}{\partial z} \qquad \text{(A2-45)}$$

Using (A2-44) and (A2-45) in (A2-42) and collecting terms we have

$$\frac{\partial}{\partial t}\varphi_i - D\frac{\partial^2}{\partial z^2}\varphi_i - \left[\frac{\partial D}{\partial z} + D\left(-\frac{1}{H} + 2\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right]\frac{\partial \varphi_i}{\partial z}\right.$$

$$+\left[\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z}\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\left\{\frac{\partial D}{\partial z} + D\left(-\frac{1}{H}\right.\right.\right.$$

$$\left.\left.\left.+\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right)\right\} - D\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial^2 \psi}{\partial z^2} - D\left(\frac{\partial \psi}{\partial z}\right)^2\left\{-\frac{i}{\psi^2}\right.\right.$$

$$\left.\left.+\frac{(i+1)}{(\psi+1)^2}\right\} + \sum_{j=0}^{n} A_{ji}\,(1-\delta_{ij}) + P_{1,0:0,1}\,\nu n\,\{(2i+1)\,\psi + i\}\right.$$

$$\left.+ C_{1,0}\,\nu' n\,[0]\;(i\,e^{\theta/T} + i + 1)\right]\;\varphi_i = \sum_{j=0}\left\{A_{ij}\,(1+\varphi_j)\,e^{-(j-i)\theta/T_v}\right\}(1-\delta_{ij})$$

$$-\left[\left(\frac{i}{\psi} - \frac{i+1}{\psi+1}\right)\frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z}\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\left\{\frac{\partial D}{\partial z} + D\left\{-\frac{1}{H}\right.\right.\right.$$

$$\left.\left.\left.+\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right\} + \sum_{j=0} A_{ji}\,(1-\delta_{ij}) - D\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial^2 \psi}{\partial z^2}\right.\right.$$

$$\left.\left.- D\left(\frac{\partial \psi}{\partial z}\right)^2\left\{-\frac{i}{\psi^2} + \frac{i+1}{(\psi+1)^2}\right\} + P_{1,0:0,1}\,\nu n\,\{(2i+1)\,\psi + i\}\right.\right.$$

$$\left.\left.+ C_{1,0}\,\nu' n\,[0]\;(i\,e^{\theta/T} + i + 1)\right] + P_{1,0:0,1}\,\nu n\,\{(2i+1)\,\psi + i\}\right]$$

$$+ C_{1,0}\,\nu' n\,[0]\;\left[i\,e^{\theta/T_V} + (i+1)\,e^{\theta/T - \theta/T_V}\right] + \varphi_{i-1}\,e^{\theta/T_v}\left[P_{1,0:0,1}\,\nu n_i\,\psi\right.$$

$$\left.+ C_{1,0}\,\nu' n\,[0]\;i\right] + \varphi_{i+1}\,e^{-\theta/T_V}\left[P_{1,0:0,1}\,\nu n(i+1)\,(\psi+1)\right.$$

$$\left.+ C_{1,0}\,\nu' n\,[0]\;e^{\theta/T}\,(i+1)\right] \qquad \text{(A2-46)}$$

The boundary conditions for the ϵ_i's are, by assumption, identical for set 1 and set 2 boundary conditions for ψ. For

initial condition $\varphi_i(z, 0) = 0$ for all i

lower boundary $\varphi_i(120, t) = 0$ for all i

upper boundary $$\frac{\partial n_i}{\partial z} = -\frac{n_i}{H}$$

thus,

$$\frac{\partial n_i'}{\partial z} + \frac{\partial \epsilon_i}{\partial z} = -\frac{n_i'}{H} - \frac{\epsilon_i}{H}$$

using (A2-45)

$$n_i' \left[-\frac{1}{H} + \left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right] + \frac{\partial \epsilon_i}{\partial z} = -\frac{n_i}{H} - \frac{\epsilon_i}{H}$$

thus

$$n_i' \left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z} + \frac{\partial \epsilon_i}{\partial z} = -\frac{\epsilon_i}{H}$$

using equation (A2-32) we obtain

$$\left.\frac{\partial \epsilon_i}{\partial z}\right|_{z=\infty} = -\left.\frac{\epsilon_i}{H}\right|_{z=\infty}$$

now using (A2-37) and (A2-39) we have

$$n_i' \frac{\partial}{\partial z}\varphi_i + \varphi_i \frac{\partial n_i}{\partial z} = -\varphi_i \frac{n_i'}{H}$$

thus, using (A2-45)

$$n_i' \frac{\partial}{\partial z}\varphi_i + \varphi_i n_i' \left\{-\frac{1}{H} + \left(\frac{i}{\psi} - \frac{i+1}{\psi+1}\right)\frac{\partial \psi}{\partial z}\right\} = -\varphi_i \frac{n_i}{H}$$

again using (A2-32) we have

$$\left[n_i' \frac{\partial \varphi_i}{\partial z} \right]_{z=\infty} = 0$$

or

$$\left. \frac{\partial \varphi_i}{\partial z} \right|_{z=\phi} = 0 \quad \text{for all i} \tag{A2-47}$$

From equation (A2-46) it is seen that all solutions are coupled through the electronic source term and that only those levels adjacent to the level of interest are coupled through vibration-vibrational or vibrational-translational energy exchange terms. If ψ is assumed known, then equation (A2-46) represents a set of 6, coupled, linear, partial differential equations for the ϵ_i's.

APPENDIX III

CONSTRUCTION OF FINITE DIFFERENCE EQUATIONS

To numerically solve equations (A2-30) and (A2-46) we will use the finite difference approximation of Crank and Nicholson (see reference (36)). This particular choice was made because, in a linear problem, the errors are of order two in both the time and space step, and the solutions are expected to be unconditionally stable.

A3.1 Finite difference form, the ψ equation.

Equation (A2-30) becomes in six point finite difference form with

$$\psi_\ell^m = \psi((\ell - 1)\Delta z,\ (m - 1)\Delta t) \qquad \ell = 1,\ 2,\ \cdots,\ L$$

$$m = 1,\ 2,\ \cdots,\ M \qquad \text{(A3-1)}$$

where Δz is the altitudinal space step size and Δt is the time step size

$$\frac{\psi_\ell^{m+1} - \psi_\ell^m}{\Delta t} - \frac{1}{n_\ell}\left(\frac{\partial Dn}{\partial z}\right)_\ell \frac{1}{2\Delta z}\left\{\psi_{\ell+1}^m - \psi_{\ell-1}^m\right\}$$

$$- \frac{D_\ell}{2(\Delta z)^2}\left\{\psi_{\ell+1}^{m+1} - 2\psi_\ell^{m+1} + \psi_{\ell-1}^{m+1} + \psi_{\ell+1}^m - 2\psi_\ell^m + \psi_{\ell-1}^m\right\}$$

$$= \sum_{j=0} \sum_{i=0} \left[\frac{1}{\psi_{\ell+}^m + 1}\left(\frac{\psi_\ell^m}{\psi_\ell^m + 1}\right)^j + \frac{\epsilon_j}{n}\right](i - j)\, A_{ij} \qquad \text{(A3-2)}$$

and the subscript ℓ and superscript m mean that the quantities are evaluated at the altitude 120+ $(\ell$-1) Δz and time $\sum_1^m$ (m-1) Δt, respectively. The term ϵ_j /n has been retained in the source term in (A3-2) for completeness. Solving for the m+1 superscripted terms in (A3-2) we have

$$- \frac{D_\ell \Delta t}{2(\Delta z)^2} \psi_{\ell+1}^{m+1} + \left\{1 + \frac{D_\ell \Delta t}{(\Delta z)^2}\right\} \psi_\ell^{m+1} - \frac{D_\ell \Delta t}{2(\Delta z)^2} \psi_{\ell-1}^{m+1}$$

$$= \left\{\frac{D_\ell \Delta t}{2(\Delta z)^2} + \frac{1}{n_\ell}\left(\frac{\partial Dn}{\partial z}\right)_\ell \frac{\Delta t}{2\Delta z}\right\} \psi_{\ell+1}^m$$

$$+ \left\{1 - \frac{D_\ell \Delta t}{(\Delta z)^2}\right\} \psi_\ell^m + \left\{\frac{D_\ell \Delta t}{2(\Delta z)^2} - \frac{1}{n_\ell}\left(\frac{\partial Dn}{\partial z}\right)_\ell \frac{\Delta t}{2\Delta z}\right\} \psi_{\ell-1}^m$$

$$+ \Delta t \sum_{j=0} \sum_{i=0} \left[\frac{1}{\psi_\ell^m + 1}\left(\frac{\psi_\ell^m}{\psi_\ell^m + 1}\right)^j + \frac{\ell \epsilon_j^m}{n}\right] (i - j) A_{ij} \quad \text{(A3-3)}$$

Let

$$A_\ell = \frac{D_\ell \Delta t}{2(\Delta z)^2} \quad \text{(A3-4)}$$

$$B_\ell = 1 + \frac{D_\ell \Delta t}{(\Delta z)^2}$$

$$= 1 + 2 A_\ell \quad \text{(A3-5)}$$

$$D_\ell = \left\{A_\ell + \frac{1}{n_\ell}\left(\frac{\partial Dn}{\partial z}\right)_\ell \frac{\Delta t}{\Delta z}\right\} \psi_{\ell+1}^m + \{1 - 2A_\ell\} \psi_\ell^m$$

$$+ \left\{A_\ell - \frac{1}{n_\ell}\left(\frac{\partial Dn}{\partial z}\right)_\ell \frac{\Delta t}{2\Delta z}\right\} \psi_{\ell-1}^m$$

$$+ \Delta t \sum_{j=0} \sum_{i=0} \left[\frac{1}{\psi_{\ell+1}^m}\left(\frac{\psi_\ell^m}{\psi_\ell^m + 1}\right)^j + \frac{\ell \epsilon_j^m}{n}\right] (i - j) A_{ij} \quad \text{(A3-6)}$$

Thus (A3-3) becomes

$$- A_\ell \psi_{\ell+1}^{m+1} + B_\ell \psi_\ell^{m+1} - A_\ell \psi_{\ell-1}^{m+1} = D_\ell^m \quad \text{(A3-7)}$$

The boundary conditions become

		set 1	set 2	
	$m = 1$	$\psi_{\ell}^{1} = 0$	$\psi_{\ell}^{1} = 7.329241\ E - 05$	
	$\ell = 1$	$\psi_{1}^{m} = 0$	$\psi_{1}^{m} = 7.329241\ E - 05$	
(A3-8)	$\ell = L$	$\psi_{L}^{m} - \psi_{L-1}^{m} = 0$	$\psi_{L}^{m} - \psi_{L-1}^{m} = 0$	(A3-9)

A3.2 Finite difference form, the φ_i equations.

Let

$$\ell\alpha_{i}^{m} = \left[\frac{\partial D}{\partial z} + D\left(-\frac{1}{H} + 2\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right)\right]_{\ell,m} \tag{A3-10}$$

$$\begin{aligned}\ell\beta_{i}^{m} = \Bigg[&\left(\frac{i}{\psi} - \frac{i+1}{\psi+1}\right)\frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z}\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\left\{\frac{\partial D}{\partial z}\right.\\ &\left. + D\left(-\frac{1}{H} + \left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial \psi}{\partial z}\right)\right\} - D\left\{\frac{i}{\psi} - \frac{i+1}{\psi+1}\right\}\frac{\partial^2 \psi}{\partial z^2}\\ &- D\left(\frac{\partial \psi}{\partial z}\right)^2\left\{-\frac{i}{\psi^2} + \frac{(i+1)}{(\psi+1)^2}\right\} + \sum_{j=0} A_{ij}\,(1 - \delta_{ij})\\ &+ P_{1,0:0,1}\,\nu n\{(2i+1)\,\psi + i\} + C_{1,0}\,\nu' n[0]\,(i e^{\theta/T} + i + 1)\Bigg]_{\ell,m}\end{aligned} \tag{A3-11}$$

$$\begin{aligned}\ell\gamma_{i}^{m} = \Bigg[&\sum_{j=0}\left\{A_{ij}\,(1 + \varphi_j)\,e^{-(j-i)\,\theta/T_V}\,(1 - \delta_{ij}) - \ell\beta_{i}^{m}\right.\\ &+ P_{1,0:0,1}\,\nu n\,\{(2i+1)\,\psi + i\} + C_{1,0}\,\nu' n[0]\left\{i\,e^{\theta/T_V}\right.\\ &\left.\left. + (i+1)\,e^{\theta/T - \theta/T_V}\right\} + \varphi_{i-1}\,e^{\theta/T_V}\,[P_{1,0:0,1}\,\nu n i\psi\right.\\ &+ C_{1,0}\,\nu' n[0]\,i] + \varphi_{i+1}\,e^{-\theta/T_V}\,[P_{1,0:0,1}\,\nu n(i+1)\,(\psi+1)\\ &\left. + C_{1,0}\,\nu' n[0]\,e^{\theta/T}\,(i+1)]\right]_{\ell m}\end{aligned} \tag{A3-12}$$

Using (A3-10) through (A3-12) and expressing (A2-46) in finite difference form we have after some rearrangement of terms

$$- \frac{D_\ell \Delta t}{2(\Delta z)^2} {}_{\ell+1}\varphi_i^{m+1} + \left[\frac{D_\ell \Delta t}{(\Delta z)^2} + 1\right] {}_\ell\varphi_i^{m+1} - \frac{D_\ell \Delta t}{2(\Delta z)^2} {}_{\ell-1}\varphi_i^{m+1}$$

$$= \left[\frac{D_\ell \Delta t}{2(\Delta z)^2} + {}_\ell\alpha_i^m \frac{\Delta t}{2\Delta z}\right] {}_{\ell+1}\varphi_i^m + \left[1 - \frac{D_\ell \Delta t}{(\Delta z)^2}\right.$$

$$\left. - {}_\ell\beta_i^m \Delta t\right] {}_\ell\varphi_i^m + \left[\frac{D_\ell \Delta t}{2(\Delta z)^2} - {}_\ell\alpha_i^m \frac{\Delta t}{2\Delta z}\right] {}_{\ell-1}\varphi_i^m$$

$$+ {}_\ell\gamma_i^m \Delta t \qquad \text{(A3-13)}$$

Let

$${}_\ell A_i = \frac{D_\ell \Delta t}{2(\Delta z)^2} \qquad \text{(A3-14)}$$

$${}_\ell B_i = 1 + \frac{D_\ell \Delta t}{(\Delta z)^2} \qquad \text{(A3-15)}$$

$$= 1 + 2\,{}_\ell A_i$$

$${}_\ell C_i^m = \left[\frac{D_\ell \Delta t}{2(\Delta z)^2} + {}_\ell\alpha_i^m \frac{\Delta t}{2\Delta z}\right] {}_{\ell+1}\varphi_i^m + \left[1 - \frac{D_\ell \Delta t}{(\Delta z)^2} - {}_\ell\beta_i^m \Delta t\right] {}_\ell\varphi_i^m \qquad \text{(A3-16)}$$

$$+ \left[\frac{D_\ell \Delta t}{2(\Delta z)^2} - {}_\ell\alpha_i^m \frac{\Delta t}{2\Delta z}\right] {}_{\ell-1}\varphi_i^m + {}_\ell\gamma_i^m \Delta t$$

Thus equation (A3-13) becomes

$$- {}_\ell A_i^{\lambda+1}\, \varphi_i^{m+1} + {}_\ell B_i\, {}_\ell\varphi_i^{m+1} - {}_\ell A_i\, {}_{\ell-1}\varphi_i^{m+1} = {}_\ell C_i^m \qquad \text{(A3-17)}$$

The boundary conditions are

$$
\begin{array}{lll}
m = 1 & {}^{\ell}\varphi_i^1 = 0 & \text{for all } i \\
\ell = 1 & {}^{1}\varphi_i^m = 0 & \text{for all } i \\
\ell = L & {}^{L}\varphi_i^m - {}^{L-1}\varphi_i^m = 0 & \text{for all } i
\end{array}
\qquad \text{(A3-18)}
$$

APPENDIX IV

COMPUTER PROGRAM LISTINGS

BOLTSOL

```
C  THIS PROGRAM CALCULATES THE                                                00000100
C    VIBRATIONAL TEMPERATURE, AND NUMBER DENSITY                             00000200
C   OF VIBRATIONAL QUANTA PRODUCED BY SLOW ELECTRON                          00000300
C   COLLISIONS FOR VIBRATIONAL NITROGEN.                                     00000400
C  THE SYMBOLOGY IS THAT CONTAINED IN THE ANALYTICAL                         00000500
C     FORMULATION OF THE PROBLEM.                                            00000600
C  THE DIMENSIONS OF PSI WILL CHANGE WITH THE UPPER ALTITUDE                 00000700
C     LIMIT,ZUPPER,THE STEP SIZE,DELZ.                                       00000800
C   TIMEX IS THE MAXIMUM TIME AND DELT IS THE TIME STEP.                     00000900
C  PSI SHOULD BE DIMENSIONED ACCORDING TO PSI(IALT, 2    ) WHERE            00001000
C     MINIMUM VALUE  OF IALT IS                                              00001100
C           IALT = 1. + (ZUPPER - 120.)/DELZ                                 00001200
C   IPMOVE IS (ARRAY SIZE)*BYTES*(NUMBER OF ARRAYS).                         00001300
C  ALL OTHER ARRAYS ARE DIMENSIONED FOR A 10. KM. DELZ.                      00001400
C   MMMTIN GOVERNS THE PRINTER LISTING AND PLOTTING FREQUENCY.               00001500
C   TCHANG IS THE TIME AT WHICH THE STEP SIZE IS CHANGED                     00001600
C     TO DELT2 FROM DELT.                                                    00001700
C   ITFLAG IS A FLAG TO INDICATE TO THE PROGRAM THAT MORE                    00001800
C     THAN ONE TIME STEP IS USED.                                            00001900
C   IFLAG IS RELATED TO ITFLAG AND IS INITIALLY SET TO ZERO.                 00002000
C   ICFLAG IS A FLAG TO INDICATE TO THE PROGRAM THAT A CORRECTION            00002100
C     USING RESULTS FROM PROGRAM BOLTDEV IS TO BE APPLIED TO                 00002200
C     THE SOURCE TERM OF THIS PROGRAM.                                       00002300
      REAL *4 NED,NI,INT,NZ,NE,MBAR,N2Z,NZ1,NZ2,MBAR1,MBAR2,NOZ              00002400
      LOGICAL*1 IMAGE(5151)                                                  00002500
      DIMENSION RAID(8),TED(80),ZD(10),NED(45)                               00002600
     C     ,GAMIZD(70),W(15),X(15),Y(15),ZP(15)                              00002700
     C     ,ID1(15),ID2(15),Z(89),NOZ(89),RATEOE(89),RATEOD(89)              00002800
     C     ,TEI(2),TE(89),NZ(6),NE(89),A(89)                                 00002900
     C     ,NZ1(6),NZ2(6),P1(6,6),P2(6,6),P3(6,6),P4(6,6)                    00003000
     C     ,INT(6,6),E(10),B(89),C(89),D1(89),D2(89)                         00003100
     C     ,D3(89),       D(89),DI(89),PSI(89,2)                             00003200
     C    ,EC(89),F(89),TV(90),QUANTA(89),N2Z(89)                           00003300
     C     ,TZZ(89),        ALPSI(90),GRID(8281),CORR(89)                    00003400
     C     ,ALN2Z(89),ALNE(89),ALQUAN(89),DSOUR(89),DSOURC(89),TV1(1)       00003500
     X     ,PHI(6,21),EPSIL(6,21),NBOLT(6,21),SUMC(6,6),G(1),N2Z1(1)        00003600
C  DATA INPUT.                                                               00003700
      READ (5,1,END=90000) RAID                                              00003800
    1 FORMAT (F5.1)                                                          00003900
      WRITE (6,2)RAID                                                        00004000
    2 FORMAT ('1',8F6.1)                                                     00004100
      READ (5,3,END=90000) TED                                               00004200
    3 FORMAT (F6.0)                                                          00004300
      WRITE (6,4) TED                                                        00004400
    4 FORMAT ('0',10F7.0)                                                    00004500
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      READ (5,5,END=90000) ZD                                          00004600
    5 FORMAT (F5.0)                                                    00004700
      WRITE (6,6) ZD                                                   00004800
    6 FORMAT ('0',10F6.0)                                              00004900
      READ (5,7,END=90000) NED                                         00005000
    7 FORMAT (E11.5)                                                   00005100
      WRITE (6,8) NED                                                  00005200
    8 FORMAT ('0',10E12.5)                                             00005300
      READ (5,10,END=90000) GAMIZD                                     00005400
   10 FORMAT (E13.7)                                                   00005500
      WRITE (6,11) GAMIZD                                              00005600
   11 FORMAT ('0',8E14.7)                                              00005700
      READ (5,12,END=90000) DELZ,ZUPPER,DELT,TIMEX,MMMTIN,ITFLAG       00005800
     X     ,TCHANG,DELT2,ICFLAG,RATEO                                  00005900
   12 FORMAT (F4.0,F5.0,F6.0,F7.0,I4,I2,F7.0,F6.0,I2,E10.2)            00006000
      WRITE (6,13)DELZ,ZUPPER,DELT,TIMEX,MMMTIN,ITFLAG,TCHANG,DELT2,   00006100
     X    ICFLAG,RATEO                                                00006200
   13 FORMAT ('0',F4.0,F5.0,F6.0,F7.0,I4,I2,F7.0,F6.0,I2,E10.2)        00006300
      READ (5,14,END=90000) DII,TI,NI,ENU,TOO                          00006400
   14 FORMAT (F6.4,F6.0,E13.7,F5.3,F5.0)                               00006500
      WRITE (6,15) DII,TI,NI,ENU,TOO                                   00006600
   15 FORMAT ('0',F6.4,F6.0,E13.7,F5.3,F5.0)                           00006700
      READ (5,16,END=90000) E                                          00006800
   16 FORMAT ((1X,F6.4))                                               00006900
      WRITE (6,17) E                                                   00007000
   17 FORMAT ('0',10(1X,F6.4))                                         00007100
      READ (5,18,END=90000) (W(N),X(N),Y(N),ZP(N),                     00007200
     C           ID1(N),ID2(N),N=1,15)                                 00007300
   18 FORMAT (1X,4E14.6,3X,2I1)                                        00007400
      WRITE (6,19) (W(N),X(N),Y(N),ZP(N),ID1(N),ID2(N),N=1,15)         00007500
   19 FORMAT ('0',1X,4E14.6,3X,2I1)                                    00007600
      READ (5,20,END=90000) RAI                                        00007700
   20 FORMAT (F5.1)                                                    00007800
      WRITE (6,21) RAI                                                 00007900
   21 FORMAT ('0',F5.1)                                                00008000
C RECONSTRUCTION OF THE INTEGRATED CHEN CROSS-SECTIONS                 00008100
C     PARAMETERS.                                                      00008200
      WRITE (6,26)                                                     00008300
   26 FORMAT ('0',2X,'ID',2X,'III',2X,'JJJ',8X,'P1',9X,'P2',           00008400
     C          13X,'P3',12X,'P4')                                     00008500
      DO 2700 IM=1,15                                                  00008600
      III = ID1(IM) + 1                                                00008700
      JJJ = ID2(IM) + 1                                                00008800
      P1(III,JJJ) = W(IM)                                              00008900
      P2(III,JJJ) = X(IM)                                              00009000
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      P3(III,JJJ) = Y(IM)                                              00009100
      P4(III,JJJ) = ZP(IM)                                             00009200
 2700 WRITE (6,27) ID1(IM),ID2(IM),III,JJJ,P1(III,JJJ)                 00009300
     C     ,P2(III,JJJ),P3(III,JJJ),P4(III,JJJ)                       00009400
   27 FORMAT ('0',2X,2I1,3X,I1,3XI1,1P4E14.6)                         00009500
C  TEST OF RAI  FOR TABLE RANGE.                                      00009600
      DO 2100 I=1,7                                                    00009700
      I1 = I                                                           00009800
 2100 IF (RAI.GE.RAID(I).AND.RAI.LT.RAID(I+1)) GO TO 2300              00009900
      WRITE (6,22)                                                     00010000
   22 FORMAT ('1','RAI NOT WITHIN TABLE RANGE')                        00010100
      WRITE (6,23) RAI                                                 00010200
   23 FORMAT ('0',F6.1)                                                00010300
      STOP                                                             00010400
 2300 CONTINUE                                                         00010500
C SET DIAGONAL ELEMENTS OF INTEGRATED CROSS-SECTION MATRIX             00010600
C     TO ZERO.                                                         00010700
      DO 2900 IIK=1,6                                                  00010800
 2900 INT(IIK,IIK) = 0.                                                00010900
      IPMOVE = 89*4*1                                                  00011000
      IFLAG = 0                                                        00011100
      MLOW = 2                                                         00011200
      BK = 8.61703E-05                                                 00011300
      THETA = 3380.                                                    00011400
      MMAX = TCHANG/DELT                                               00011500
      MMMIN = 0                                                        00011600
      DIFI =(DII*NI)/(TI**0.75)                                        00011700
      CALL JACH2 (Z,TOO,TZ,NZ,MBAR,RHOZ,HZ)                            00011800
C  CALCULATION OF TIME INVARIANT COEFFICIENTS AT EACH                  00011900
C     VERTICAL GRID POINT.                                             00012000
      LMAX = 1 + (ZUPPER - 120.)/DELZ                                  00012100
 3900 WRITE (6,41)                                                     00012200
   41 FORMAT ('0',5X,'DIFF',10X,'A',12X,'B',12X,'C',12X,               00012300
     C    'D1',12X,'D2',10X,'D3', 5X,'L')                             00012400
      DO 2000  L=1,LMAX                                                00012500
      Z(L) = 120. + (L -1)*DELZ                                        00012600
C  TEST OF Z TO BE WITHIN TABLE RANGES.                                00012700
      DO 2400 K=1,9                                                    00012800
 2400 IF (Z(L).GE.ZD(K).AND.Z(L).LT.ZD(K+1)) GO TO 2500                00012900
      WRITE (6,24)                                                     00013000
   24 FORMAT ('1','ALTITUDE IS NOT WITHIN TABLE RANGE')                00013100
      WRITE (6,25) Z(L)                                                00013200
   25 FORMAT ('0', F5.0)                                               00013300
      STOP                                                             00013400
 2500 IK = K                                                           00013500
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      IL = K + 1                                                        00013600
C CALCULATION OF TEI.                                                   00013700
C TEI INDEX  IS THE LINE NUMBER.                                        00013800
C OF THE PLOTTED ELECTRON TEMPERATURE DATA.                             00013900
      DO 2600 LL=1,2                                                    00014000
 2600 TEI(LL) = GAMIZD(IK + 10*(II-1) + LL - 1)                         00014100
     C    *(RAI - RAID(II)) + TED((II-1)*10 +IK+LL-1)                   00014200
C  CALCULATION OF BETAZI AND THE ELECTRON TEMPERATURE.                  00014300
      BETAZI = (TEI(2) - TEI(1))/(ZD(IL) - ZD(IK))                      00014400
      TE(L) = BETAZI*(Z(L) - ZD(IK)) + TEI(1)                           00014500
C  CALCULATION OF ELECTRON DENSITY.                                     00014600
      DO 100 IT=1,44                                                    00014700
      ZTEST1 = 20.*(IT-1) + 120.                                        00014800
      ZTEST2 = ZTEST1 + 20.                                             00014900
      IF ( Z(L).GE.ZTEST1.AND.Z(L).LE.ZTEST2) GO TO 200                 00015000
  100 CONTINUE                                                          00015100
      WRITE (6,51)                                                      00015200
   51 FORMAT ('0','ALTITUDE FOR NE CALCULATION IS OUTSIDE TABLE')       00015300
      WRITE (6,52) Z(L)                                                 00015400
   52 FORMAT ('0',2X,F6.0)                                              00015500
      STOP                                                              00015600
  200 ITT = IT                                                          00015700
      GRADNE = (NED(ITT+1) - NED(ITT))/20.                              00015800
      NE(L) = GRADNE*(Z(L) - ZTEST1) + NED(ITT)                         00015900
      ZA = Z(L)                                                         00016000
      CALL JACH2(ZA,TOO,TZ,NZ,MBAR,RHOZ,HZ)                             00016100
      N2Z(L) = NZ(1)                                                    00016200
      NOZ(L) = NZ(3)                                                    00016201
      SUMNZ = NZ(1)  + NZ(3)                                            00016300
      TZZ(L) = TZ                                                       00016400
      RATEOD(L) = RATEO*NOZ(L)                                          00016401
      RATEOE(L) = RATEOD(L)*EXP(-THETA/TZZ(L))                          00016402
C CALCULATION OF DIFFUSION,A AND B COEFFICIENTS.                        00016500
      DIFF = DIFI*(TZ**0.75)/SUMNZ                                      00016600
      A(L) = (DIFF * DELT)/(2. *((DELZ*1.E+05)**2.))                    00016700
      B(L) = 1. + 2.*A(L)                                               00016800
      IF(L.EQ.1) GO TO 2000                                             00016900
C  CALCULATION OF DERIVATIVE OF PRODUCT OF DIFFUSION                    00017000
C     COEFFICIENT AND MOLECULAR NITROGEN DENSITY                        00017100
C     WITH RESPECT TO ALTITUDE.                                         00017200
      Z1 = Z(L) - 0.5*DELZ                                              00017300
      Z2 = Z(L) + 0.5*DELZ                                              00017400
      CALL JACH2 (Z1,TOO,TZ1,NZ1,MBAR1,RHOZ1,HZ1)                       00017500
      CALL JACH2 (Z2,TOO,TZ2,NZ2,MBAR2,RHOZ2,HZ2)                       00017600
      SUMNZ1 = NZ1(1) + NZ1(3)                                          00017700
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      SUMNZ2 = NZ2(1) + NZ2(3)                                          00017800
      DIFF1 = DIFI*(TZ1**0.75)/SUMNZ1                                   00017900
      DIFF2 = DIFI*(TZ2**0.75)/SUMNZ2                                   00018000
      DERIV = (DIFF2*NZ2(1) - DIFF1*NZ1(1))/(DELZ*1.E+05)               00018100
C  CALCULATION OF C AND TIME INDEPENDENT PARTIAL D COEFFICIENTS.        00018200
      C(L) = (DERIV*DELT)/(2.*(DELZ*1.E+05)*NZ(1))                      00018300
      D1(L) = A(L) + C(L)                                               00018400
      D2(L) = 1. - 2.*A(L)                                              00018500
      D3(L) = A(L) - C(L)                                               00018600
      WRITE (6,42) DIFF,A(L),B(L),C(L),D1(L),D2(L),D3(L),L              00018700
   42 FORMAT ('0',1P7E13.5,I3)                                          00018800
 2000 CONTINUE                                                          00018900
      C(1) = C(2)                                                       00019000
      D1(1) = A(1) + C(1)                                               00019100
      D2(1) = 1. - 2.*A(1)                                              00019200
      D3(1) = A(1) - C(1)                                               00019300
      WRITE (6,61)                                                      00019301
   61 FORMAT ('1',2X,'ALT',6X,'RATEOE',8X,'RATEOD',5X,'N(O)')           00019302
      WRITE (6,62) (Z(ILN),RATEOE(ILN),RATEOD(ILN),NOZ(ILN),ILN=1,LMAX) 00019303
   62 FORMAT ('0',0PF5.0,1P3E13.5)                                      00019304
      IF (IFLAG.EQ.1) GO TO 3950                                        00019400
C  CALCULATION OF EC AND F COEFFICIENTS FOR INITIAL TIME STEP.          00019500
C  LLL IS THE ALTITUDE STEP INDEX.                                      00019600
      EC(1) = 0.                                                        00019700
      F(1) = 7.329241E-05                                               00019800
      WRITE (6,43)                                                      00019900
   43 FORMAT ('1',6X,'DI',10X,'EC',10X,'F',10X,'DENOM',10X,'LLL')       00020000
      DO 3200 LLL=1,LMAX                                                00020100
C    SET DSOURC TO ZERO.                                                00020200
      DSOURC(LLL) = 0.                                                  00020300
C  CALCULATION OF INTEGRATED CHEN CROSS-SECTION VALUES                  00020400
C     AT ALTITUDE OF INTEREST.                                           00020500
      BKTE = BK*TE(LLL)                                                 00020600
      RTE = 1./TE(LLL)                                                  00020700
      RTE2 = RTE*RTE                                                    00020800
      RTE3 = RTE2*RTE                                                   00020900
      DO 2800 IN=1,15                                                   00021000
      IIJ = ID1(IN) + 1                                                 00021100
      JJI = ID2(IN) + 1                                                 00021200
      INT (IIJ,JJI) = EXP(P1(IIJ,JJI) + P2(IIJ,JJI)*RTE                 00021300
     C     + P3(IIJ,JJI)*RTE2 + P4(IIJ,JJI)*RTE3)                       00021400
 2800 INT(JJI,IIJ) = INT(IIJ,JJI)*EXP(-(E(JJI) - E(IIJ))/BKTE)          00021500
C CALCULATION OF INITIAL SOURCE TERM DI.                                00021600
      SUMSI = 0.                                                        00021700
      DO 3400 IIL = 1,6                                                 00021800
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      SUM = (IIL-1)*INT(IIL,1)*NE(LLL)                                  00021900
 3400 SUMSI = SUMSI + SUM                                               00022000
      DI(LLL) = SUMSI*DELT + RATEOE(LLL)*DELT*(F(1) + 1. -              00022100
     X               F(1)*EXP(THETA/TZZ(LLL)))                          00022101
C  END CALCULATION OF INITIAL SOURCE TERM AT ALTITUDE DENOTED BY LLL.    00022200
      IF (LLL.EQ.1) GO TO 3200                                          00022300
      DENOM = B(LLL) - A(LLL)*EC(LLL- 1)                                00022400
      EC(LLL)= A(LLL)/DENOM                                             00022500
      F(LLL) = (DI(LLL) + A(LLL)*F(LLL -1))/DENOM                       00022600
      WRITE (6,44) DI(LLL),EC(LLL),F(LLL),DENOM,LLL                     00022700
   44 FORMAT ('0',1P4E13.6,I3)                                          00022800
 3200 CONTINUE                                                          00022900
C  CALCULATION OF INITIAL PSI.                                          00023000
      MMM = 1                                                           00023100
      LLMAX = LMAX - 1                                                  00023200
      PSI(LMAX-1,1) = F(LMAX-1)/(1.-EC(LMAX-1))                         00023300
      DO 3500 NNN=2,LLMAX                                               00023400
      NNNN = LMAX - NNN                                                 00023500
      PSI(NNNN,1) = EC(NNNN)*PSI(NNNN+1,1) + F(NNNN)                    00023600
      NNNNA = NNNN  + 1                                                 00023700
      TV(NNNNA) = THETA/ALOG((PSI(NNNNA, 1 )+1.)/PSI(NNNNA, 1 ))       00023800
      QUANTA(NNNNA) = N2Z(NNNNA)*PSI(NNNNA, 1 )                         00023900
 3500 CONTINUE                                                          00024000
      PSI(LMAX,1) = PSI(LMAX - 1,1)                                     00024100
      PSI(LMAX+1,1) = PSI(LMAX,1)                                       00024200
      TV(LMAX  ) = THETA/ALOG((PSI(LMAX  , 1 )+1.)/PSI(LMAX  , 1 ))     00024300
      TV(1) = 0.                                                        00024400
      QUANTA(1) = 0.                                                    00024500
      QUANTA(LMAX  ) = N2Z(LMAX  )*PSI(LMAX  , 1 )                      00024600
C   WRITE RESULTS ON OUTPUT TAPE.                                       00024700
      WRITE (10) (Z(ILN),TZZ(ILN),TE(ILN),TV(ILN),N2Z(ILN),NE(ILN),     00024800
     C     QUANTA(ILN),PSI(ILN, 1 ),DI(ILN),D(ILN),MMM,DELZ,            00024900
     X     MMAX,DELT,IFLAG,ILN=1,LMAX)                                  00025000
      WRITE (6,34)                                                      00025100
   34 FORMAT ('1',2X,'ALT',          2X,'T',6X,'TE',                    00025200
     C    4X,'TV', 4X,'N(N2)', 8X,'NE', 12X,'QUANTA',                   00025300
     C     9X,'PSI', 5X,'SOURCE INT',5X,'SOURCE',5X,'ELEC SOURCE',      00025400
     X   2X,'CORRECTION')                                               00025500
      WRITE (6,35) MMM,MMAX,DELT,IFLAG,ICFLAG,MMMIN                     00025600
   35 FORMAT ('0',6X,I4,6X,I4,6X,F6.0,6X,I2,I2,I4)                      00025700
      WRITE (6,28) (Z(IKN),TZZ(IKN),TE(IKN),TV(IKN),N2Z(IKN),NE(IKN)    00025800
     C    ,QUANTA(IKN),PSI(IKN, 1 ),DI(IKN),D(IKN),DSOUR(IKN),          00025900
     X   DSOURC(IKN),IKN=1,LMAX)                                        00026000
   28 FORMAT (' ',0PF5.0,0P3F6.0,1P8E13.5)                              00026100
C  CALCULATION OF COEFFICIENTS AND PSI FOR OTHER TIME STEPS.            00026200
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C MMMT IS AN INDEX CONTROLLING THE AMOUNT OF PRINTED OUTPUT.                00026300
C  MMM IS THE TIME STEP INDEX.                                              00026400
      MMMT = 2                                                             00026500
      IF (ICFLAG.EQ.0) GO TO 3950                                          00026600
      READ (11,END=90001,ERR=90002)  MMMIN,DELT1,LBOUND,DELZ1,DELZ2,       00026700
     X  LINC,(G(1),N2Z1(1),TV1(1),(I,PHI(I,ILN),EPSIL(I,ILN),              00026800
     X   NBOLT(I,ILN),I=1,6,1),ILN=1,LMAX)                                 00026900
 3950 DO 3600 MMM=MLOW,MMAX                                                00027000
      DO 3700 LLLL=1,LMAX                                                  00027100
      IF (LLLL.EQ.1) D(1)=D1(1)*PSI(2,  1  )+DI(1)                         00027200
      IF (LLLL.EQ.1) GO TO 3700                                            00027300
C  CALCULATION OF INTEGRATED CHEN CROSS-SECTION VALUES                     00027400
C     AT ALTITUDE OF INTEREST.                                            00027500
      BKTE = BK*TE(LLLL)                                                   00027600
      RTE = 1./TE(LLLL)                                                    00027700
      RTE2 = RTE*RTE                                                       00027800
      RTE3 = RTE2*RTE                                                      00027900
      DO 3801 IJK=1,15                                                     00028000
      INI = ID1(IJK) + 1                                                   00028100
      INJ = ID2(IJK) + 1                                                   00028200
      INT(INI,INJ) = EXP(P1(INI,INJ) + P2(INI,INJ)*RTE                     00028300
     C     + P3(INI,INJ)*RTE2 + P4(INI,INJ)*RTE3)                          00028400
 3801 INT(INJ,INI) = INT(INI,INJ)*EXP(-(E(INJ) - E(INI))/BKTE)             0002
C  CALCULATION OF D COEFFICIENT AT ALTITUDE LLLL.                          0002
      SUMST = 0.                                                           0002
      DO 3901 IIII=1,6                                                     0002
      DO 3901 JJJJ=1,6                                                     0002
      SUMS = 1./(PSI(LLLL, 1  ) + 1.)*((PSI(LLLL, 1  )/                    0002
     C   (PSI(LLLL,  1  )+1.))**(JJJJ-1))*(IIII-JJJJ)                      0002
     C   *INT(IIII,JJJJ)*NE(LLLL)                                          0002
 3901 SUMST = SUMST + SUMS                                                 0002
      IF (ICFLAG.EQ.0) GO TO 1500                                          0002
 1100 IF(MMM-MMMIN)1500,1200,90003                                         0002
 1200 SUMT = 0.                                                            0002
      DO 1300 II=1,6                                                       0002
      DO 1300 JJ=1,6                                                       0002
      SUMC(II,JJ) = INT(II,JJ)*NE(LLLL)*EPSIL(JJ,LLLL)*(II-JJ)             0002
 1300 SUMT = SUMT + SUMC(II,JJ)                                            0003
      CORR(LLLL) = SUMT/N2Z(LLLL)                                          0003
      DSOURC(LLLL) = CORR(LLLL)*DELT                                       0003
      IF (LLLL.EQ.LMAX) GO TO 1000                                         0003
      GO TO 1600                                                           0003
 1000 READ (11,END=90001,ERR=90002)  MMMIN,DELT1,LBOUND,DELZ1,DELZ2,       0003
     X  LINC,(G(1),N2Z1(1),TV1(1),(I,PHI(I,ILN),EPSIL(I,ILN),              0003
     X   NBOLT(I,ILN),I=1,6,1),ILN=1,LMAX)                                 0003
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      GO TO 1600                                                        00030800
 1500 DSOURC(LLLL) = 0.                                                 00030900
 1600 CONTINUE                                                          00031000
      DSOUR(LLLL) = SUMST*DELT + DSOURC(LLLL)                           00031100
      D(LLLL) = D1(LLLL)*PSI(LLLL+1,  1  ) + D2(LLLL)*PSI(LLLL,  1  )   00031200
     C     + D3(LLLL)*PSI(LLLL-1,  1  ) + DSOUR(LLLL)                   00031300
     X     + RATEOE(LLLL)*DELT*(PSI(LLLL,1) + 1.                        00031301
     X     -    PSI(LLLL,1)*EXP(THETA/TZZ(LLLL)))                       00031302
      DENOM1 = B(LLLL) - A(LLLL)*EC(LLLL-1)                             00031400
      EC(LLLL)= A(LLLL)/DENOM1                                          00031500
      F(LLLL) = (D(LLLL) + A(LLLL)*F(LLLL-1))/DENOM1                    00031600
 3700 CONTINUE                                                          00031700
C   CALCULATION OF PSI, VIBRATIONAL TEMPERATURE,ETC.                    00031800
      PSI(LMAX-1, 2 ) = F(LMAX-1)/(1.-EC(LMAX-1))                       00031900
      PSI(LMAX, 2 ) = PSI(LMAX-1, 2 )                                   00032000
      PSI(LMAX+1, 2 ) = PSI(LMAX, 2 )                                   00032100
      DO 4000 INN=2,LLMAX                                               00032200
      NNNNN = LMAX - INN                                                00032300
      PSI(NNNNN, 2 ) = EC(NNNNN)*PSI(NNNNN+1, 2 ) + F(NNNNN)            00032400
      NNNNM = NNNNN + 1                                                 00032500
      TV(NNNNM) = THETA/ALOG((PSI(NNNNM, 2 )+1.)/PSI(NNNNM, 2 ))        00032600
 4000 QUANTA(NNNNM) = N2Z(NNNNM)*PSI(NNNNM, 2 )                         00032700
      TV(LMAX  ) = THETA/ALOG((PSI(LMAX  , 2 )+1.)/PSI(LMAX  , 2 ))     00032800
      TV(1) = 0.                                                        00032900
      QUANTA(1) = 0.                                                    00033000
      QUANTA(LMAX  ) = N2Z(LMAX  )*PSI(LMAX  , 2 )                      00033100
C   WRITE RESULTS ON OUTPUT TAPE.                                       00033200
      WRITE (10) (Z(ILN),TZZ(ILN),TE(ILN),TV(ILN),N2Z(ILN),NE(ILN),     00033300
     C     QUANTA(ILN),PSI(ILN, 2 ),DI(ILN),D(ILN),MMM,DELZ,            00033400
     X     MMAX,DELT,IFLAG,ILN=1,LMAX)                                  00033500
C   TEST FOR PRINTING AND PLOTTING.                                     00033600
      IF(MMM.NE.MMMT) GO TO 3600                                        00033700
      MMMT = MMMT + MMMTIN                                              00033800
      WRITE (6,34)                                                      00033900
      WRITE (6,35) MMM,MMAX,DELT,IFLAG,ICFLAG,MMMIN                     00034000
      WRITE (6,28) (Z(IKN),TZZ(IKN),TE(IKN),TV(IKN),N2Z(IKN),NE(IKN)    00034100
     C    ,QUANTA(IKN),PSI(IKN, 2 ),DI(IKN),D(IKN),DSOUR(IKN),          00034200
     C         DSOURC(IKN),IKN=1,LMAX)                                  00034300
C CONSTRUCTION OF PRINTER PLOTTER ARRAYS.                               00034400
      DO 4100 IMN=2,LMAX                                                00034500
      ALPSI(IMN) = ALOG10(PSI(IMN, 2 ))                                 00034600
      ALN2Z(IMN) = ALOG10(N2Z(IMN))                                     00034700
      ALQUAN(IMN) = ALOG10(QUANTA(IMN))                                 00034800
 4100 ALNE(IMN) = ALOG10(NE(IMN))                                       00034900
C PRINTER PLOTTING.                                                     00035000
```

```
      WRITE (6,29)                                                      00035100
   29 FORMAT ('1',46X,'TEMPERATURES VERSUS ALTITUDE')                   00035200
      XR = 1000.                                                        00035300
      XL = 0.                                                           00035400
      YT = 10000.                                                       00035500
      YB = 0.                                                           00035600
      NUMPR1 = LMAX + 1                                                 00035700
      NUMPR2 = LMAX                                                     00035800
      CALL PLOT2 (GRID,XR,XL,YT,YB)                                     00035900
      CALL PLOT3 ('T',Z,TZZ,NUMPR1)                                     00036000
      CALL PLOT3 ('V',Z,TV,NUMPR1)                                      00036100
      CALL PLOT4 (20,'TEMPERATURE  DEG. K ')                            00036200
      WRITE (6,30)                                                      00036300
   30 FORMAT('0',59X,'ALTITUDE (KM.)')                                  00036400
      WRITE (6,31)                                                      00036500
   31 FORMAT ('1',51X,'PSI VERSUS ALTITUDE')                            00036600
      YT = 0.0                                                          00036700
      YB = -5.0                                                         00036800
      CALL PLOT2 (GRID,XR,XL,YT,YB)                                     00036900
      CALL PLOT3 ('*',Z,ALPSI,NUMPR2)                                   00037000
      CALL PLOT4 (3,'PSI')                                              00037100
      WRITE (6,30)                                                      00037200
      YT = +9.0                                                         00037300
      YB = +4.0                                                         00037400
      WRITE (6,32)                                                      00037500
   32 FORMAT ('1',46X,'QUANTA AND ELECTRON DENSITIES')                  00037600
      CALL PLOT2 (GRID,XR,XL,YT,YB)                                     00037700
      CALL PLOT3 ('E',Z,ALNE,NUMPR2)                                    00037800
      CALL PLOT3 ('Q',Z,ALQUAN,NUMPR2)                                  00037900
      CALL PLOT4 (23,'NUMBER DENSITY CM**-3  ')                         00038000
      WRITE (6,30)                                                      00038100
 3600 CALL CMOVE(IPMOVE,PSI(1,2),1,PSI(1,1),1)                          00038200
      CONTINUE                                                          00038300
C    TEST FOR CHANGE OF TIME STEP.                                      00038400
      MLOW = MMAX + 1                                                   00038500
      IF (ITFLAG.EQ.1.AND.IFLAG.EQ.0) GO TO 3800                        00038600
      END FILE 10                                                       00038700
      STOP                                                              00038800
C    SET UP DO LOOP INDICIES FOR SECOND TIME INCREMENT STEP SIZE.       00038900
 3800 DELT = DELT2                                                      00039000
      MMAX = (TIMEX - TCHANG)/DELT2 + MLOW - 1                          00039100
      IFLAG = ITFLAG                                                    00039200
      GO TO 3900                                                        00039300
90000 WRITE (6,33)                                                      00039400
   33 FORMAT ('1','END OF FILE ENCOUNTERED ON CARD READER')             00039500
```

```
      STOP                                                              00039600
90001 WRITE (6,84)                                                      00039700
   84 FORMAT ('1','END OF FILE ENCOUNTERED ON INPUT TAPE')              00039800
      STOP                                                              00039900
90002 WRITE (6,85)                                                      00040000
   85 FORMAT ('1','IO ERROR ENCOUNTERED ON INPUT TAPE')                 00040100
      STOP                                                              00040200
90003 WRITE (6,86)                                                      00040300
   86 FORMAT ('1','MMMIN  IS LESS THAN MMM')                            00040400
      STOP                                                              00040500
      END                                                               00040600
                                                                              041C CA
```

BOLTDEV

```
C  THIS PROGRAM CALCULATES THE DEPARTURES IN NUMBER DENSITY                00000100
C     FROM A BOLTZMAN DISTRIBUTION OF VIBRATIONAL QUANTA                   00000200
C     PRODUCED BY AN ELECTRONIC SOURCE.                                    00000300
C  THE SYMBOLOGY IS THAT CONTAINED IN THE ANALYTICAL                       00000400
C     FORMULATION OF THE PROBLEM.                                          00000500
C  THE DIMENSIONS OF PSI WILL CHANGE WITH THE UPPER ALTITUDE               00000600
C      LIMIT,ZUPPER,THE STEP SIZE,DELZ,THE MAXIMUM TIME,TIMEX,             00000700
C      AND THE TIME STEP SIZE,DELT.                                        00000800
C  PHI SHOULD BE DIMENSIONED ACCORDING TO PHI(6,IALT) WHERE                00000900
C      MINIMUM VALUE  OF IALT IS                                           00001000
C            IALT = 1. + (ZUPPER - 120.)/DELZ                              00001100
C  ALL OTHER ARRAYS ARE DIMENSIONED FOR A 10. KM. DELZ.                    00001200
C   MMMT IS AN INDEX CONTROLLING THE AMOUNT OF PRINTED OUTPUT.             00001300
C   MMMTIN GOVERNS THE PRINTER LISTING AND PLOTTING FREQUENCY.             00001400
C   ISTART IS THE TIME STEP FROM BOLTSOL RESULTS AT WHICH THE              00001500
C      CALCULATIONS OF DEVIATIONS IS STARTED.                              00001600
C   LINC CONTROLS THE ALTITUDE INCREMENT FOR THE DEVIATION                 00001700
C     PART OF THE PROGRAM,  EQUIVALENT DELZ =LINC*DELZ                     00001800
C   DELZ IS THE ALTITUDE INCREMENT FOR THE BOLTZMAN PART                   00001900
C      OF THE PROBLEM.                                                     00002000
C   DELT IS THE TIME INCREMENT FOR THE BOLTZMAN PART                       00002100
C     OF THE PROBLEM.                                                      00002200
C   EDELT IS THE EQUIVALENT TIME STEP FOR THE DEVIATION                    00002300
C     PART OF THE PROBLEM.                                                 00002400
C   TINC IS THE NUMBER OF DELT INCREMENTS IN EDELT.                        00002500
C   LBOUND IS THE LOWER BOUNDARY FOR THE DEVIATION CALCULATION.            00002600
      REAL *4 NED,NI,INT,NZ,NE,MBAR,N2Z,NZ1,NZ2,MBAR1,MBAR2,NU,NBOLT      00002700
     X        ,NOZ                                                         00002701
      INTEGER TINC,TINC2                                                  00002800
      LOGICAL*1 IMAGE(5151)                                               00002900
      DIMENSION Z(89),RAID(8),TED(80),ZD(10),NED(45)                      00003000
     X ,GAMIZD(70),      NZ(6),NE(89),A(89),NOZ(89)                       00003100
     X  ,W(15),X(15),Y(15),ZP(15),ID1(15)                                 00003101
     X  ,ID2(15),TEI(2),TE(89),P1(6,6)                                    00003102
     X  ,P2(6,6),P3(6,6),P4(6,6),INT(6,6)                                 00003103
     X    ,NZ1(6),NZ2(6),GRADT(89),HPRESS(89)                             00003200
     X             ,E(10),B(89),MMAX1(3),DELT1(3),IFLAG(3),               00003300
     X     N2Z(89), MMM(3),DI(89),PSI(30,3),RATEOE(89),RATEOD(89)         00003400
     X    ,TZZ(89),GRID(8281),SUME1A(89),SUME2A(89)                       00003500
     X    ,DERIVD(89),DIFF(89),H(89),DPSIZ(89),DPSIT(89)                  00003600
     X    ,D2PSIZ(89),ALPHA(6,89),BETA(6,89),GAMMA(6,89)                  00003700
     X    ,NU(89),P1001(89),TV(30,3)   ,QUANTA(30,1),D(30,1)              00003800
     X    ,PHI(6,89),C1(6,89),C2(6,89),C3(6,89),C(6,89),F(6,89)           00003900
     X    ,EC(6,89),ALPHI1(89),ALPHI2(89),ALPHI3(89),ALPHI4(89),          00004000
     X    ALPHI5(89),ALPHI6(89),EPSIL(6,89),NBOLT(6,89),REPSIL(6,89)      00004100
```

```
C  DATA INPUT.                                                          00004200
      READ (5,1,END=90000) RAID                                         00004201
    1 FORMAT (F5.1)                                                     00004202
      WRITE (6,2)RAID                                                   00004203
    2 FORMAT ('1',8F6.1)                                                00004204
      READ (5,3,END=90000) TED                                          00004205
    3 FORMAT (F6.0)                                                     00004206
      WRITE (6,4) TED                                                   00004207
    4 FORMAT ('0',10F7.0)                                               00004208
      READ (5,5,END=90000) ZD                                           00004209
    5 FORMAT (F5.0)                                                     00004210
      WRITE (6,6) ZD                                                    00004211
    6 FORMAT ('0',10F5.0)                                               00004212
      READ (5,7,END=90000) NED                                          00004213
    7 FORMAT (E11.5)                                                    00004214
      WRITE (6,8) NED                                                   00004215
    8 FORMAT ('0',10E12.5)                                              00004216
      READ (5,10,END=90000) GAMIZD                                      00004217
   10 FORMAT (E13.7)                                                    00004218
      WRITE (6,11) GAMIZD                                               00004219
   11 FORMAT ('0',8E14.7)                                               00004220
      READ (5,12,END=90000) DELZ,ZUPPER,DELT,TIMEX,MMMTIN,LINC,TINC     00004700
     X     ,LBOUND,TINC2,RATEO                                          00004800
   12 FORMAT (F4.0,F5.0,F6.0,F7.0,I4,4I3,E10.2)                         00004900
      WRITE (6,13)DELZ,ZUPPER,DELT,TIMEX,MMMTIN,LINC,TINC               00005000
     X    ,LBOUND,TINC2,RATEO                                          00005100
   13 FORMAT ('0',F4.0,F5.0,F6.0,F7.0,I4,4I3,E10.2)                     00005200
      READ (5,14,END=90000) DII,TI,NI,ENU,TOO                           00005300
   14 FORMAT (F6.4,F6.0,E13.7,F5.3,F5.0)                                00005400
      WRITE (6,15) DII,TI,NI,ENU,TOO                                    00005500
   15 FORMAT ('0',F6.4,F6.0,E13.7,F5.3,F5.0)                            00005600
      READ (5,16,END=90000) E                                           00005700
   16 FORMAT ((1X,F6.4))                                                00005800
      WRITE (6,17) E                                                    00005900
   17 FORMAT ('0',10(1X,F6.4))                                          00006000
      READ (5,18,END=90000) (W(N),X(N),Y(N),ZP(N),                      00006001
     C            ID1(N),ID2(N),N=1,15)                                00006002
   18 FORMAT (1X,4E14.6,3X,2I1)                                         00006003
      WRITE (6,19) (W(N),X(N),Y(N),ZP(N),ID1(N),ID2(N),N=1,15)          00006004
   19 FORMAT ('0',1X,4E14.6,3X,2I1)                                     00006005
      READ (5,20,END=90000) RAI                                         00006006
   20 FORMAT (F5.1)                                                     00006007
      WRITE (6,21) RAI                                                  00006008
   21 FORMAT ('0',F5.1)                                                 00006009
      READ (5,22) ISTART                                                00006100
```

```
   22 FORMAT (I4)                                                        00006200
      WRITE (6,23) ISTART                                                00006300
   23 FORMAT ('0',I4)                                                    00006400
      CALL JACH2(Z,TOO,TZ,NZ,MBAR,RHOZ,HZ)                              00006500
C RECONSTRUCTION OF THE INTEGRATED CHEN CROSS-SECTIONS                   00006501
C     PARAMETERS.                                                        00006502
      WRITE (6,26)                                                       00006503
   26 FORMAT ('0',2X,'ID',2X,'III',2X,'JJJ',8X,'P1',9X,'P2',             00006504
     C         13X,'P3',12X,'P4')                                        00006505
      DO 2700 IM=1,15                                                    00006506
      III = ID1(IM) + 1                                                  00006507
      JJJ = ID2(IM) + 1                                                  00006508
      P1(III,JJJ) = W(IM)                                                00006509
      P2(III,JJJ) = X(IM)                                                00006510
      P3(III,JJJ) = Y(IM)                                                00006511
      P4(III,JJJ) = ZP(IM)                                               00006512
 2700 WRITE (6,27) ID1(IM),ID2(IM),III,JJJ,P1(III,JJJ),                  00006513
     X     P2(III,JJJ),P3(III,JJJ),P4(III,JJJ)                          00006514
   27 FORMAT ('0',2X,2I1,2(3X,I1),1P4E14.6)                              00006515
      DIFI =(DII*NI)/(TI**0.75)                                          00006600
C    IPMOV AND IMMOV ARE  (ARRAY SIZE)*BYTES*(NUMBER OF ARRAYS)          00006700
      IPMOV = 30*4*2                                                     00006800
      IMMOV = 1*4*2                                                      00006900
      BK = 8.61703E-05                                                   00007000
      THETA = 3380.                                                      00007100
      ISTAR = ISTART - 1                                                 00007200
      LMAX = 1. + (ZUPPER - 120.)/DELZ                                   00007300
C    SET PHI(I,L),EC(I,LBOUND),AND F(I,LBOUND) TO ZERO.                  00007400
C    SET REPSIL(I,LBOUND) AND DIAGONAL ELEMENTS OF THE                   00007401
C      INTEGRATED CHEN CROSS-SECTION MATRIX TO ZERO.                     00007402
      DO 3000 IJ = 1,6                                                   00007500
      DO 3001 K=1,LBOUND                                                 00007600
      EC(IJ,K) = 0.                                                      00007700
 3001 F(IJ,K) = 0.                                                       00007800
      REPSIL(IJ,LBOUND) = 0.                                             00007900
      INT(IJ,IJ) = 0.                                                    00007901
      DO 3000 LL = 1,LMAX,LINC                                           00008000
 3000 PHI(IJ,LL) = 0.                                                    00008100
C    READ TAPE CONTAINING BOLTZMAN PART SOLUTION.                        00008200
      READ ( 10,END=90001,ERR=90002)   (Z(ILN),TZZ(ILN),TE(ILN),         00008300
     X             TV(ILN,1),N2Z(ILN),NE(ILN),QUANTA(ILN,1),           00008400
     X     PSI(ILN,1),DI(ILN),D(ILN,1),MMM(1),DELZ1,                   00008500
     X      MMAX1(1),DELT1(1),IFLAG(1),ILN=1,LMAX)                     00008600
      IF (ISTAR - MMM(1)) 90003,3600,4100                                00008700
 3600 DO 3700 M=2,3                                                      00008800
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```
 3700 READ ( 10,END=90001,ERR=90002)   (Z(ILN),TZZ(ILN),TE(ILN),          00008900
     X            TV(ILN,M),N2Z(ILN),NE(ILN),QUANTA(ILN,1),              00009000
     X     PSI(ILN,M),DI(ILN),D(ILN,1),MMM(M),DELZ1,                     00009100
     X      MMAX1(M),DELT1(M),IFLAG(M),ILN=1,LMAX)                       00009200
      MMMT = ISTAR + 1                                                  00009300
      GO TO 6000                                                        00009400
 4100 DO 1000 JK=3,ISTAR                                                00009500
 1000 READ (10,END=90001,ERR=90002)                                     00009600
      MMMT = ISTART + 1                                                 00009700
      DO 4200 LM=1,3                                                    00009800
 4200 READ ( 10,END=90001,ERR=90002)   (Z(ILN),TZZ(ILN),TE(ILN),         00009900
     X            TV(ILN,LM),N2Z(ILN),NE(ILN),QUANTA(ILN,1),            00010000
     X     PSI(ILN,LM),DI(ILN),D(ILN,1),MMM(LM),DELZ1,                   00010100
     X      MMAX1(LM),DELT1(LM),IFLAG (LM),ILN=1,LMAX)                   00010200
      GO TO 6000                                                        00010300
 3900 DO 3901 J=1,TINC                                                  00010400
      CALL CMOVE (IPMOV,PSI(1,2),1,PSI(1,1),1)                          00010500
      CALL CMOVE (IPMOV,TV(1,2),1,TV(1,1),1)                            00010600
      CALL CMOVE(IMMOV,MMM(2),1,MMM(1),1)                               00010700
      CALL CMOVE(IMMOV,MMAX1(2),1,MMAX1(1),1)                           00010800
      CALL CMOVE(IMMOV,DELT1(2),1,DELT1(1),1)                           00010900
      CALL CMOVE(IMMOV,IFLAG(2),1,IFLAG(1),1)                           00011000
      READ ( 10,END=90001,ERR=90002)   (Z(ILN),TZZ(ILN),TE(ILN),        00011100
     X            TV(ILN,3),N2Z(ILN),NE(ILN),QUANTA(ILN,1),             00011200
     X     PSI(ILN,3),DI(ILN),D(ILN,1),MMM(3),DELZ1,                     00011300
     X      MMAX1(3),DELT1(3),IFLAG(3),ILN=1,LMAX)                       00011400
      IF (IFLAG (3).EQ.1.AND.IFLAG (2).EQ.0) GO TO 6000                 00011500
 3901 CONTINUE                                                          00011600
      GO TO 3800                                                        00011700
C  CALCULATION OF A,B AND OTHER TIME INVARIANT TERMS.                   00011800
 6000 DELT = DELT1(3)                                                   00011900
      IF (IFLAG(3).EQ.1) TINC = TINC2                                   00012000
      EDELT = DELT*TINC                                                 00012100
      DO 2500 II=1,LMAX,LINC                                            00012400
      CALL JACH2 (Z(II),TOO,TZ,NZ,MBAR,RHOZ,HZ)                         00012500
      HPRESS(II) = HZ*MBAR/28.                                          00012600
      NOZ(II) = NZ(3)                                                   00012601
      SUMNZ = NZ(1) + NZ(3)                                             00012700
      DIFF(II) = DIFI*(TZ**0.75)/SUMNZ                                  00012800
      A(II) =(DIFF(II)*EDELT)/(2.*((DELZ*LINC*1.E+05)**2.))             00012900
      B(II) = 1. + 2*A(II)                                              00013000
      T05=TZ**0.5                                                       00013100
      NU(II) = 1.48209E-11*T05                                          00013200
      P1001(II) = 2.6003E-06*TZ*EXP(91.5/TZ)                            00013300
      RATEOD(II) = RATEO*NOZ(II)                                        00013301
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      RATEOE(II) = RATEOD(II)*EXP(-THETA/TZZ(II))                          00013302
C  CALCULATION OF DERIVATIVES OF DIFF.,TEMP. AND DENSITY SCALE HEIGHT.     00013400
      IF (II.EQ.1) GO TO 2500                                              00013500
      Z1 = Z(II) -0.5*DELZ                                                 00013600
      Z2 = Z(II) + 0.5*DELZ                                                00013700
      CALL JACH2(Z1,TOO,TZ1,NZ1,MBAR1,RHOZ1,HZ1)                           00013800
      CALL JACH2 ( Z2,TOO,TZ2,NZ2,MBAR2,RHOZ2,HZ2)                         00013900
      GRADT(II) = (TZ2 - TZ1)/DELZ                                         00013901
      H(II) = HPRESS(II)/(1 + HPRESS(II) * GRADT(II)/TZZ(II))              00013902
      SUMNZ1 = NZ1(1) + NZ1(3)                                             00014000
      SUMNZ2 = NZ2(1) + NZ2(3)                                             00014100
      DIFF1 = DIFI*(TZ1**0.75)/SUMNZ1                                      00014200
      DIFF2 = DIFI*(TZ2**0.75)/SUMNZ2                                      00014300
      DERIVD (II) = (DIFF2 - DIFF1)/(DELZ*1.E+05)                          00014400
 2500 CONTINUE                                                             00014500
      GRADT(1) = GRADT(2)                                                  00014501
      H(1) = HPRESS(1)/(1 + HPRESS(1) * GRADT(1)/TZZ(1) )                  00014502
      DERIVD(1) = DERIVD(2)                                                00014600
      LINCP1 = LINC + LBOUND                                               00014700
      LLMAX = LMAX - LINC                                                  00014800
      MMMAX = MMAX1(3) - 1                                                 00014900
 3800 DO 4000 L = LINCP1,LLMAX,LINC                                        00015000
C   CALCULATION OF DERIVATIVES OF PSI WITH RESPECT TO                      00015100
C      ALTITUDE AND TIME.                                                 00015200
      DPSIZ(L) = (PSI(L+1,2) - PSI(L-1,2))/(2.*(DELZ*1.E+05))              00015300
      D2PSIZ(L) = (PSI(L+1,2) -2.*PSI(L,2) + PSI(L-1,2))/                  00015400
     X      ((DELZ*1.E+05)**2 )                                           00015500
      DELTS = DELT1(1) + DELT1(3)                                          00015600
      DPSIT(L) = (PSI(L,3  ) - PSI(L,  1))/(2.*DELTS)                      00015700
C  CALCULATION OF INTEGRATED CHEN CROSS-SECTION VALUES                     00015701
C      AT ALTITUDE OF INTEREST.                                           00015702
      BKTE = BK*TE(L)                                                      00015703
      RTE = 1./TE(L)                                                       00015704
      RTE2 = RTE*RTE                                                       00015705
      RTE3 = RTE2*RTE                                                      00015706
      DO 2800 IN=1,15                                                      00015707
      IIJ = ID1(IN) + 1                                                    00015708
      JJI = ID2(IN) + 1                                                    00015709
      INT (IIJ,JJI) = EXP(P1(IIJ,JJI) + P2(IIJ,JJI)*RTE                    00015710
     C      + P3(IIJ,JJI)*RTE2 + P4(IIJ,JJI)*RTE3)                        00015711
 2800 INT(JJI,IIJ) = INT(IIJ,JJI)*EXP(-(E(JJI) - E(IIJ))/BKTE)             00015712
      DO 4000 I=1,6                                                        00015800
      BRAKET = (I-1)/PSI(L,2) - I/(PSI(L,2) + 1.)                          00015900
      ALPHA(I,L) = DERIVD(L) + DIFF(L)*(-1./(H(L)*1.E+05) + 2.*BRAKET      00016000
     X         *DPSIZ(L))                                                00016100
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C   CALCULATION OF SOURCE TERMS.                                          00016200
C  CALCULATION OF SUMMATIONS FOR USE IN BETA AND GAMMA.                   00016201
      SUMA1 = 0.                                                         00016202
      SUMA2 = 0.                                                         00016203
      DO 5000 IIL=1,6                                                    00016204
      SUM1 = INT(I,IIL)*NE(L)                                            00016205
      SUMA1 = SUMA1 + INT(IIL,I)*NE(L)                                   00016206
      SUM2 = SUM1*(1. + PHI(IIL,L))*EXP( (I - IIL)*THETA/TV(L,2))        00016207
 5000 SUMA2 = SUMA2 + SUM2                                               00016208
      BETA(I,L) = BRAKET*DPSIT(L) - DPSIZ(L)*BRAKET*(DERIVD(L) +         00016900
     X    DIFF(L)*(-1./(H(L)*1.E+05) + BRAKET*DPSIZ(L)))                 00017000
     X   - DIFF(L)*BRAKET*D2PSIZ(L) - DIFF(L)*(DPSIZ(L)**2 )*(-(I-1)/    00017100
     X   (PSI(L,2)**2 ) + I/((PSI(L,2) + 1.)**2 ))                       00017200
     X   + SUMA1 + P1001(L)*NU(L)*N2Z(L)*((2.*I - 1.)*PSI(L,2) + I -1.)  00017300
     X   + RATEOE(L)*((I-1)*EXP(THETA/TZZ(L)) + (I-1) + 1.)              00017301
      IF (I.EQ.1) GO TO 7000                                             00017400
      IF (I.EQ.6) GO TO 8000                                             00017500
      GAMMA (I,L) = SUMA2 - BETA(I,L) + P1001(L)*NU(L)*N2Z(L)*((         00017600
     X   2.*I - 1.)*PSI(L,2) + I - 1. + (I-1.)*PSI(L,2)*PHI(I-1,L)      00017700
     X   *EXP(THETA/TV(L,2)) + I*(PSI(L,2) + 1.)*PHI(I+1,L)             00017800
     X   *EXP(-THETA/TV(L,2)))                                          00017900
     X   + RATEOE(L)*((I-1)*EXP(THETA/TV(L,2))*(PHI(I-1,L) + 1.) +      00017901
     X    I*EXP(THETA/TZZ(L) - THETA/TV(L,2))*(PHI(I+1,L) + 1.))        00017902
      GO TO 4500                                                         00018000
 7000 GAMMA(I,L) = SUMA2 - BETA(I,L) + P1001(L)*NU(L)*N2Z(L)*((          00018100
     X   2.*I - 1.)*PSI(L,2) + I - 1. + I*(PSI(L,2) + 1.)*PHI(2,L)      00018200
     X   *EXP(-THETA/TV(L,2)))                                          00018300
     X   + RATEOE(L)*EXP(THETA/TZZ(L) - THETA/TV(L,2))*(PHI(2,L) + 1.)  00018301
      GO TO 4500                                                         00018400
 8000 GAMMA(I,L) = SUMA2 - BETA(I,L) + P1001(L)*NU(L)*N2Z(L)*((          00018500
2    X   2.*I - 1.)*PSI(L,2) + I - 1. + (I - 1.)*PSI(L,2)*PHI(I-1,L)    00018600
     X   *EXP(THETA/TV(L,2)))                                           00018700
     X   + RATEOE(L)*(I-1)*EXP(THETA/TV(L,2))*(PHI(I-1,L) + 1.)         00018701
 4500 CONTINUE                                                          00018800
      C1(I,L) = A(L) +ALPHA(I,L)*EDELT/(2.*DELZ*LINC*1.E+05)            00018900
      C2(I,L) = 1. - 2.*A(L) -BETA(I,L)*EDELT                           00019000
      C3(I,L) = A(L) -ALPHA(I,L)*EDELT/(2.*DELZ*LINC*1.E+05)            00019100
      C(I,L) = C1(I,L)*PHI(I,L+LINC)+C2(I,L)*PHI(I,L)+ C3(I,L)          00019200
     X   *PHI(I,L-LINC)+GAMMA(I,L)*EDELT                                00019300
C   CALCULATION OF EC(I,L) AND F(I,L) COEFFICIENTS.                     00019400
      DENOM = B(L) - A(L)*EC(I,L-LINC)                                  00019500
      EC(I,L) = A(L)/DENOM                                              00019600
      F(I,L) = (C(I,L) + A(L)*F(I,L-LINC))/DENOM                        00019700
 4000 CONTINUE                                                          00019800
C  CALCULATION OF PHI.                                                  00019900
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      IF (LBOUND.EQ.1) GO TO 4300                                       00020000
      DO 4301 IL=1,6                                                    00020100
      NBOLT(IL,LBOUND) = N2Z(LBOUND)*(1./(PSI(LBOUND,2) + 1.))*         00020200
     X       ((PSI(LBOUND,2)/(PSI(LBOUND,2) + 1.))**(IL - 1))           00020300
 4301 EPSIL(IL,LBOUND) = 0.                                             00020400
      GO TO 4400                                                        00020500
 4300 NBOLT(1,1) = N2Z(1)                                               00020600
      NBOLT(2,1) = 0.                                                   00020700
      NBOLT(3,1) = 0.                                                   00020800
      NBOLT(4,1) = 0.                                                   00020900
      NBOLT(5,1) = 0.                                                   00021000
      NBOLT(6,1) = 0.                                                   00021100
      EPSIL(1,1) = 0.                                                   00021200
      EPSIL(2,1) = 0.                                                   00021300
      EPSIL(3,1) = 0.                                                   00021400
      EPSIL(4,1) = 0.                                                   00021500
      EPSIL(5,1) = 0.                                                   00021600
      EPSIL(6,1) = 0.                                                   00021700
 4400 DO 4600 II=1,6                                                    00021800
      PHI(II,LLMAX ) = F(II,LLMAX   )/(1. - EC(II,LLMAX   ))            00021900
      PHI(II,LMAX) = PHI(II,LLMAX   )                                   00022000
      NBOLT(II,LLMAX) = N2Z(LLMAX)*(1./(PSI(LLMAX,2) + 1.))             00022100
     X   *((PSI(LLMAX,2)/(PSI(LLMAX,2) + 1.))**(II-1))                  00022200
      NBOLT(II, LMAX) = N2Z( LMAX)*(1./(PSI( LMAX,2) + 1.))             00022300
     X  *((PSI(LMAX,2)/(PSI(LMAX,2) + 1.))**(II - 1))                   00022400
      EPSIL(II,LLMAX ) = PHI(II,LLMAX )*NBOLT(II,LLMAX)                 00022500
      EPSIL(II,LMAX  ) = PHI(II,LMAX  )*NBOLT(II,LMAX)                  00022600
      LLLMAX = LMAX - 2*LINC                                            00022700
      DO 4700 LL=LINCP1,LLLMAX,LINC                                     00022800
      NN = LMAX - LINC + LBOUND - LL                                    00022900
      PHI(II,NN) = EC(II,NN)*PHI(II,NN+LINC)+F(II,NN)                   00023000
      NBOLT(II,NN   ) = N2Z(NN   )*(1./(PSI(NN   ,2) + 1.))             00023100
     X   *((PSI(NN   ,2)/(PSI(NN   ,2) + 1.))**(II-1))                  00023200
 4700 EPSIL(II,NN    ) = PHI(II,NN    )*NBOLT(II,NN)                    00023300
 4600 CONTINUE                                                          00023301
C    WRITE RESULTS TO TAPE                                              00023400
      WRITE (11)  MMM(3),DELT1(3),LBOUND,DELZ,DELZ1,LINC,(Z(ILN),       00023401
     X   N2Z(ILN),TV(ILN,2),(I,PHI(I,ILN),EPSIL(I,ILN),                 00023402
     X    NBOLT(I,ILN),I=1,6,1),ILN=LBOUND,LMAX,LINC)                   00023404
      IF (MMM(2).NE.MMMT) GO TO 3500                                    00023405
      DO 5200 NN=LBOUND,LMAX,LINC                                       00023900
      SUME1 = 0.                                                        00024000
      SUME2 = 0.                                                        00024100
      DO 5100 IK=1,6                                                    00024200
      SUME = EPSIL(IK,NN)                                               00024300
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      SUMEI = EPSIL(IK,NN)*(IK-1)                                                00024400
      SUMEl = SUMEl + SUME                                                       00024500
 5100 SUME2 = SUME2 + SUMEI                                                      00024600
      SUMElA(NN) = SUMEl                                                         00024700
      SUME2A(NN) = SUME2                                                         00024800
      IF (NN.EQ.LBOUND) GO TO 5200                                               00024900
      DO 5200 IK=1,6                                                             00025000
      REPSIL(IK,NN) = SUMElA(NN)/EPSIL(IK,NN)                                    00025100
 5200 CONTINUE                                                                   00025200
      MMMT = MMMT + MMMTIN                                                       00025400
   91 FORMAT ('1',2X,'C1(I,L)',2X,'C2(I,L)',2X,'C3(I,L)',5X,'C(I,L)',            00025500
     X    2X,'GAMMA(I,L)',             1X,'ALPHA(I,L)',1X,'BETA(I,L)',          00025600
     X    4X,'A(L)',4X,'B(L)',5X,'EC(I,L)',4X,'F(I,L)')                         00025700
      DO 4900 IJK=1,6                                                            00025800
      WRITE (6,91)                                                               00025900
      WRITE (6,92)(C1(IJK,L),C2(IJK,L),C3(IJK,L),C(IJK,L),GAMMA(IJK,L),          00026000
     X    ALPHA(IJK,L),BETA(IJK,L),A(L),B(L),EC(IJK,L),F(IJK,L),                00026100
     X     L=LINCP1,LLMAX,LINC)                                                 00026200
   92 FORMAT (' ',1P11E10.3)                                                     00026300
      WRITE (6,93)                                                               00026400
   93 FORMAT ('0',2X,'DPSIT',5X,'DERIVD',4X,'DPSIZ',5X,'D2PSIZ',8X               00026500
     X ,'DIFF',5X,'H',8X,'P1001',4X,'NU')                                        00026600
      WRITE (6,94) (DPSIT(L),DERIVD(L),DPSIZ(L),D2PSIZ(L),DIFF(L),H(L)           00026700
     X      ,P1001(L),NU(L),L=LINCP1,LLMAX,LINC)                                00026800
   94 FORMAT (' ',1P8E10.3)                                                      00026900
      WRITE (6,37)                                                               00027000
   37 FORMAT ('0',2X,'MMM',1X,'LEVEL',3X,'DELT',3X,'EDELT')                      00027100
      WRITE (6,35) MMM(3),IJK,DELT,EDELT                                         00027200
   35 FORMAT ('0',2X,I4,3X,I3,3X,F5.0,3X,F5.0)                                   00027300
      WRITE (6,34)                                                               00027400
   34 FORMAT ('0',2X,'ALT',2X,'T',          4X,'TV',                             00027500
     X      9X,'N(N2)',          8X,'PSI',11X,'PHI',8X,'SUM EPSILON',           00027600
     X      3X,'SUM I*EPSILON',3X,'EPSILON',4X,'BOLTDEN',3X,'REPSIL')           00027700
 4900 WRITE (6,36) (Z(IKN),TZZ(IKN),          TV(IKN,2),                       00027800
     X      N2Z(IKN),         PSI(IKN,2),PHI(IJK,IKN),SUMElA(IKN),              00027900
     X      SUME2A(IKN),EPSIL(IJK,IKN),NBOLT(IJK,IKN),REPSIL(IJK,IKN),         00028000
     X      IKN=LBOUND,LMAX,LINC)                                               00028100
   36 FORMAT (' ',0PF5.0,0P2F6.0,1P5E14.6,1P3E12.3)                              00028200
C    CONSTRUCITON OF PRINTER PLOTTER ARRAYS.                                    00028300
      DO 4800 JJ=LBOUND,LMAX                                                     00028400
      ALPHI1(JJ) = PHI(1,JJ)                                                     00028500
      ALPHI2(JJ) = PHI(2,JJ)                                                     00028600
      ALPHI3(JJ) = PHI(3,JJ)                                                     00028700
      ALPHI4(JJ) = PHI(4,JJ)                                                     00028800
      ALPHI5(JJ) = PHI(5,JJ)                                                     00028900
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 4800 ALPHI6(JJ) = PHI(6,JJ)                                            00029000
C  PRINTER PLOTTING.                                                    00029100
      WRITE (6,29)                                                      00029200
   29 FORMAT ('1',43X,'DEVIATION VERSUS ALTITUDE')                      00029300
      XR = 1000.                                                        00029400
      XL = 0.                                                           00029500
      YT = +14.                                                         00029600
      YB = -6.                                                          00029700
      NUMPR1 = LMAX + 1                                                 00029800
      CALL PLOT2(GRID,XR,XL,YT,YB)                                      00029900
      CALL PLOT3('1',Z,ALPHI1,NUMPR1)                                   00030000
      CALL PLOT3('2',Z,ALPHI2,NUMPR1)                                   00030100
      CALL PLOT3('3',Z,ALPHI3,NUMPR1)                                   00030200
      CALL PLOT3('4',Z,ALPHI4,NUMPR1)                                   00030300
      CALL PLOT3 ('5',Z,ALPHI5,NUMPR1)                                  00030400
      CALL PLOT3 ('6',Z,ALPHI6,NUMPR1)                                  00030500
      CALL PLOT4(3,'PHI')                                               00030600
      WRITE (6,30)                                                      00030700
   30 FORMAT ('0',59X,'ALTITUDE (KM.)')                                 00030800
 3500 IF (MMM(2).LT.MMMAX) GO TO 3900                                   00030900
      END FILE 11                                                       00031000
      STOP                                                              00031100
90000 WRITE (6,33)                                                      00031200
   33 FORMAT ('1','END OF FILE ENCOUNTERED ON CARD READER')             00031300
      STOP                                                              00031400
90001 WRITE (6,84)                                                      00031500
   84 FORMAT ('1','END OF FILE ENCOUNTERED ON INPUT TAPE')              00031600
      STOP                                                              00031700
90002 WRITE (6,85)                                                      00031800
   85 FORMAT ('1','IO ERROR ENCOUNTERED ON INPUT TAPE')                 00031900
      STOP                                                              00032000
90003 WRITE (6,86)                                                      00032100
   86 FORMAT ('1','ISTART IS LESS THAN OR EQUAL TO THE FIRST TIME       00032200
     X    STEP AVAILABLE')                                             00032300
      STOP                                                              00032400
      END                                                               00032500
                                                                  0396 (
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REACTRAT

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C    THIS PROGRAM CALCULATES THE REACTION RATES FOR ION-ATOM                00000100
C       INTERCHANGE BETWEEN O PLUS AND N2.                                  00000200
C    THE POPULATION OF THE VIBRATIONALLY EXCITED LEVELS                     00000300
C       OF N2 AND THE VIBRATIONAL TEMPERATURE COME FROM                     00000400
C       THE OUTPUT TAPE OF PROGRAM BOLTDEV.                                 00000500
        REAL * 4 NI,    N2Z,      NBOLT,KBOLT,KEFF,KVIBL,NLTOT,KPRIM        00000600
        LOGICAL * 1 IMAGE(5151)                                             00000700
        DIMENSION Z(89),       N2Z(89),PHI(6,89),TV(89),EPSIL(6,89)         00000800
       X    ,NBOLT(6,89),KBOLT(89),  KEFF(  89),RATIOK(21),KVIBL(6)        00000900
       X    ,ILEVEL(6),TAUN  (89),ALKBOL(21),ALKEFF(21),II(6),NLTOT(6,89)  00001000
       X    ,TAUB(89),TAUE(89),ALTAUB(21),ALTAUE(21),ALTAUN(21)            00001100
       X    ,ARRAY(21),ARRAY1(21),GRID(8281)                               00001200
C    DATA INPUT                                                             00001300
        READ (5,12,END=90000) DELZ,ZUPPER,DELT,TIMEX,MMMTIN,LINC,TINC       00001400
       X     ,LBOUND,TINC2                                                  00001500
     12 FORMAT (F4.0,F5.0,F6.0,F7.0,I4,4I3)                                 00001600
        WRITE (6,13)DELZ,ZUPPER,DELT,TIMEX,MMMTIN,LINC,TINC                 00001700
       X    ,LBOUND,TINC2                                                  00001800
     13 FORMAT ('0',F4.0,F5.0,F6.0,F7.0,I4,4I3)                             00001900
        READ (5,14,END=90000) DII,TI,NI,ENU,TOO                             00002000
     14 FORMAT (F6.4,F6.0,E13.7,F5.3,F5.0)                                  00002100
        WRITE (6,15) DII,TI,NI,ENU,TOO                                      00002200
     15 FORMAT ('0',F6.4,F6.0,E13.7,F5.3,F5.0)                              00002300
        READ (5,16,END=90000) (ILEVEL(N),KVIBL(N),N=1,6)                    00002400
     16 FORMAT (6(I2,E9.1))                                                 00002500
        WRITE (6,17) (ILEVEL(N),KVIBL(N),N=1,6)                             00002600
     17 FORMAT(' ',I2,E9.1)                                                 00002700
        LMAX = 1. + (ZUPPER - 120.)/DELZ                                    00002800
        READ (5,18,END=90000) INCRTM,KPRIM,IPR                              00002900
     18 FORMAT(I6,E9.1,I6)                                                  00003000
        WRITE (6,19) INCRTM,KPRIM,IPR                                       00003100
     19 FORMAT (' ',I6,1PE9.1,I6)                                           00003200
        READ (10,END=90001,ERR=90002) MMM,DELT1,LBOUND,DELZ                 00003300
       X    ,DELZ1,LINC,(Z(ILN),N2Z(ILN),TV(ILN),(II(I),                   00003400
       X    PHI(I,ILN),EPSIL(I,ILN),NBOLT(I,ILN),I=1,6,1),ILN=             00003500
       X    LBOUND,LMAX,LINC)                                              00003600
        ITEST = MMM                                                         00003700
        JMAX = INCRTM - 1                                                   00003800
        DO 1000 M=1,10000,INCRTM                                            00003900
        DO 1500 L=LBOUND,LMAX,LINC                                          00004000
        SUM1 = 0.                                                           00004100
        SUM2 = 0.                                                           00004200
        DO 2000 J=1,6                                                       00004300
        NLTOT(J,L) = NBOLT(J,L) + EPSIL(J,L)                                00004400
        A = (KVIBL(J) - KPRIM)*NBOLT(J,L)                                   00004500
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      B = KVIBL(J)*EPSIL(J,L)                                                  00004600
      SUM1 = SUM1 + A                                                          00004700
 2000 SUM2 = SUM2 + B                                                          00004800
      TAUINV = SUM1 + KPRIM*N2Z(L)                                             00004900
      TAUB(L) = 1./TAUINV                                                      00005000
      TAUE(L) = 1./(TAUINV + SUM2)                                             00005100
      TAUN  (L) = 1./(1.3E-12*N2Z(L))                                          00005200
      KBOLT(L) = KPRIM + SUM1/N2Z(L)                                           00005300
      KEFF(L) = KBOLT(L) + SUM2/N2Z(L)                                         00005400
      RATIOK(L) = KEFF(L)/KBOLT(L)                                             00005500
      ALTAUB(L) = ALOG10(TAUB(L))                                              00005600
      ALTAUE(L) = ALOG10(TAUE(L))                                              00005700
      ALTAUN(L) = ALOG10(TAUN  (L))                                            00005800
      ALKBOL(L) = ALOG10(KBOLT(L))                                             00005900
      ALKEFF(L)= ALOG10(KEFF(L))                                               00006000
 1500 CONTINUE                                                                 00006100
C   WRITE RESULTS TO TAPE.                                                     00006200
      WRITE (11) MMM,DELT1,LBOUND,DELZ,DELZ1                                   00006300
     X    ,LINC,(Z(ILN),N2Z(ILN),TV(ILN),TAUB(ILN),                           00006400
     X    TAUE(ILN),KBOLT(ILN),KEFF(ILN),RATIOK(ILN),                         00006500
     X    (II(I),  NBOLT(I,ILN),EPSIL(I,ILN),NLTOT(I,ILN),                    00006600
     X    I=1,6,1),ILN=LBOUND,LMAX,LINC)                                      00006700
      IF (MMM.NE.ITEST) GO TO 5000                                             00006800
      ITEST = ITEST + IPR                                                      00006900
      WRITE (6,20)                                                             00007000
   20 FORMAT ('1',1X,'MMM IS ')                                                00007100
      WRITE (6,21) MMM                                                         00007200
   21 FORMAT ('+',9X,I6)                                                       00007300
      WRITE (6,50)                                                             00007400
   50 FORMAT ('0',2X,'ALT',4X,'TV',4X,'N(N2)',9X,'KBOLT'9X,                    00007500
     X   'KEFF',11X,'RATIOK',7X,'TAUN',10X,'TAUB',11X,'TAUE')                 00007600
      WRITE (6,51) (Z(ILN),TV(ILN),N2Z(ILN),KBOLT(ILN),KEFF(ILN),             00007700
     X   RATIOK(ILN),TAUN(ILN),TAUB(ILN),TAUE(ILN),ILN=LBOUND,LMAX,LINC)      00007800
   51 FORMAT ('0',0PF5.0,0PF6.0,1P7E14.6)                                      00007900
C   PRINTER PLOT.                                                            00008000
      XR = 1000.                                                               00008100
      XL = 0.                                                                  00008200
      YT = 11.                                                                 00008300
      YB = 1.                                                                  00008400
      NUMPR1 = LMAX + 1                                                        00008500
      DO 3000 N=1,6                                                            00008600
      DO 3100 LL=LBOUND,LMAX,LINC                                              00008700
      IF (LL.GE.2) GO TO 3105                                                  00008800
      ARRAY(LL) = 1.                                                           00008900
      ARRAY1(LL) = 1.                                                          00009000
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      GO TO 3100                                                        00009100
 3105 ARRAY(LL) = ALOG10(NBOLT(N,LL))                                   00009200
      ARRAY1(LL) = ALOG10(NLTOT(N,LL))                                  00009300
 3100 CONTINUE                                                          00009400
      WRITE (6,22)                                                      00009500
   22 FORMAT ('1',40X,'DENSITIES VERSUS ALTITUDE FOR')                  00009600
      WRITE (6,23) N                                                    00009700
   23 FORMAT ('+',71X,I2)                                               00009800
      CALL PLOT2(GRID,XR,XL,YT,YB)                                      00009900
      CALL PLOT3('*',Z,ARRAY,NUMPR1)                                    00010000
      CALL PLOT3('+',Z,ARRAY1,NUMPR1)                                   00010100
      CALL PLOT4(27,'LOG NUMBER DENSITY (CM**-3)')                      00010200
      WRITE (6,24)                                                      00010201
   24 FORMAT ('0',59X,'ALTITUDE  (KM.)')                                00010300
 3000 CONTINUE                                                          00010400
      WRITE (6,25)                                                      00010500
   25 FORMAT ('1',40X,'REACTION RATES VERSUS ALTITUDE')                 00010600
      YT = -9.                                                          00010700
      YB = -14.                                                         00010800
      CALL PLOT2(GRID,XR,XL,YT,YB)                                      00010900
      CALL PLOT3('*',Z,ALKBOL,NUMPR1)                                   00011000
      CALL PLOT3('+',Z,ALKEF,NUMPR1)                                    00011100
      CALL PLOT4(35,'LOG REACTION RATE  (CM**3  SEC**-1)')              00011200
      WRITE (6,24)                                                      00011300
      YT = 1.5                                                          00011400
      YB = 0.5                                                          00011500
      WRITE (6,26)                                                      00011600
   26 FORMAT ('1',40X,'RATIO OF REACTION RATES')                        00011700
      CALL PLOT2(GRID,XR,XL,YT,YB)                                      00011800
      CALL PLOT3('*',Z,RATIOK,NUMPR1)                                   00011900
      CALL PLOT4(20,'RATIO OF  KEFF/KBOLT')                             00012000
      WRITE (6,24)                                                      00012100
      YT = 5.                                                           00012200
      YB = 0.                                                           00012300
      WRITE (6,27)                                                      00012400
   27 FORMAT ('1',40X,'ELECTRON LOSS TIME CONSTANT')                    00012500
      CALL PLOT 2(GRID,XR,XL,YT,YB)                                     00012600
      CALL PLOT3('*',Z,ALTAUB,NUMPR1)                                   00012700
      CALL PLOT3('+',Z,ALTAUE,NUMPR1)                                   00012800
      CALL PLOT3('N',Z,ALTAUN,NUMPR1)                                   00012900
      CALL PLOT4(24,'LOG TIME CONSTANT (SEC.)')                         00013000
 5000 IF (INCRTM.EQ.1) GO TO 5500                                       00013100
      DO 5500 JJ=1,JMAX                                                 00013200
      READ (10,END=90001,ERR=90002)                                     00013300
 5500 CONTINUE                                                          00013400
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      READ (10,END=90001,ERR=90002) MMM,DELT1,LBOUND,DELZ                00013500
     X    ,DELZ1,LINC,(Z(ILN),N2Z(ILN),TV(ILN),(II(I),                   00013600
     X    PHI(I,ILN),EPSIL(I,ILN),NBOLT(I,ILN),I=1,6,1),ILN=             00013700
     X    LBOUND,LMAX,LINC)                                              00013800
 1000 CONTINUE                                                           00013900
      END FILE 11                                                        00014000
      STOP                                                               00014100
90000 WRITE (6,33)                                                       00014200
   33 FORMAT ('1','END OF FILE ENCOUNTERED ON CARD READER')              00014300
      STOP                                                               00014400
90001 WRITE (6,84)                                                       00014500
   84 FORMAT ('1','END OF FILE ENCOUNTERED ON INPUT TAPE')               00014600
      STOP                                                               00014700
90002 WRITE (6,85)                                                       00014800
   85 FORMAT ('1','IO ERROR ENCOUNTERED ON INPUT TAPE')                  00014900
      STOP                                                               00015000
      END                                                                00015100
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